X-Lab^{Pro} 5

Operator Manual

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SOFTWARE HELP

1 Job Manager

1.1 Job Manager

The Job Manager *XLJobMan* is a module of the *X-LabPro* software package to display and edit jobs and samples.

XLJobMan contains a new tree control following the design of the Windows explorer. Using the menu entries or the command buttons of the toolbar you can create, edit, backup or delete jobs and samples. The tree control and the job window offer you context menus to do further operations. *Note:* Some menu entries and command buttons of the toolbar are disabled as long as no sample is selected or as long as no job window is opened.

1.1.1 Window overview

- Tree Control
- Job Window

Menu overview

- File Menu
- Edit Menu
- View Menu
- Job Menu
- Window Menu
- X-LabPro Menu
- Help Menu

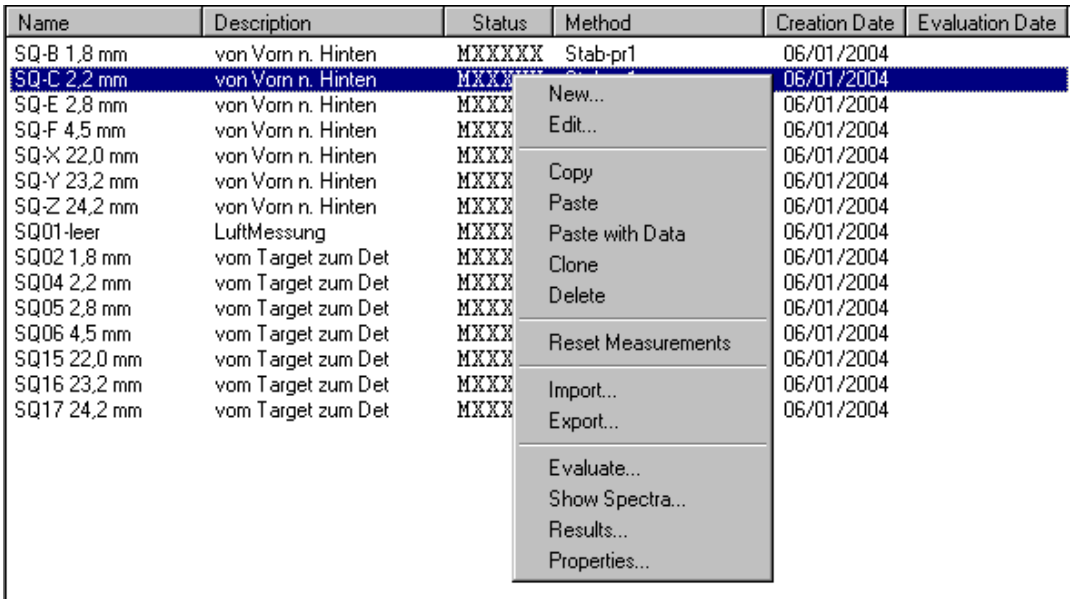
Other

- Title Bar
- Toolbar
- Status Bar

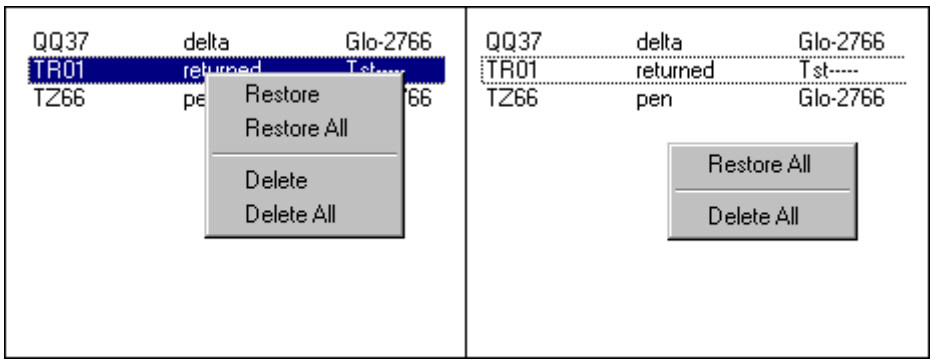
1.2 Job Window

The job window is used to display all of the samples assigned to the active job. Samples can be assigned to jobs and organized using the job window. Each customer sample has to be assigned to a job. Click on the head of a column (like in the Windows explorer) to sort the samples alternately up- and downward in relation to the contents of the selected column.

You get access to all commands of the *Edit* menu by clicking the right mouse button on a sample.



Instead of a job, the trashcan can be opened. In this case the trashcan context menu looks like shown on the following pictures.



- **Restore**
  Select *Restore* to restore the selected sample(s). The sample(s) will be assigned to the former jobs(s). If a job does not exist any more, the sample will be restored to the collective job.
- **Restore All**
  Select *Restore All* to restore all samples in the trashcan. See *Restore* for details.
- **Delete**
  Select *Delete* to delete the selected sample(s).
- **Delete All**
  Select *Delete All* to delete all samples in the trashcan.

Note:

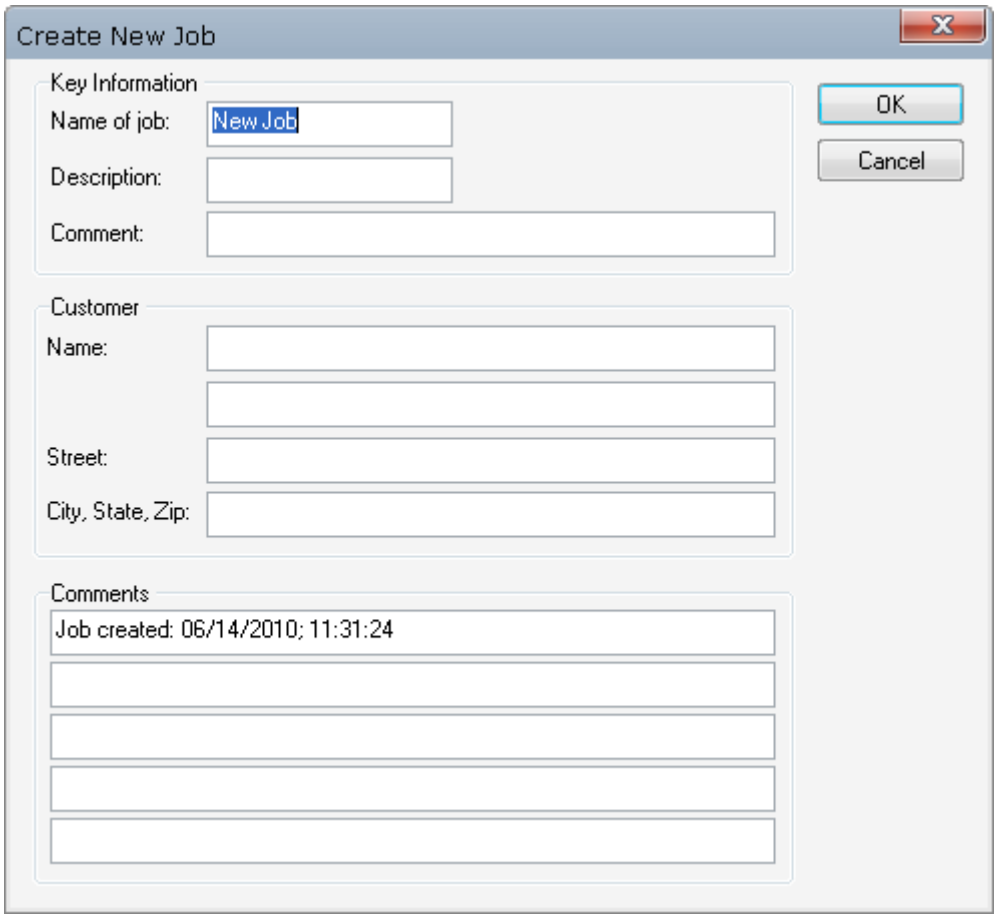
The samples should be assigned to different jobs even if your applications are not organized according to jobs. In this case, a new job may be created for each week, for example.

Changes to the data are automatically stored. Use the *New Window* menupoint of the *Window* menu or of the job context menu of the tree control to open additional job windows.

Use the *Sample* menu or the command buttons in the toolbar to copy sample data to other jobs or windows.

1.3 Create New Job/Job Properties

Use this dialog to create a new job.



Key Information Group

Name of job
Enter the name of the job to be newly created. The name may be up to 20 characters long and must be unique.

Description
Enter a description of the new job. The description may be up to 20 characters long.

Comment
Use this field to enter a comment for the new job.

Customer Group

Name
Enter the customer's name and the name of the contact person, etc. as desired in these text boxes. Up to 40 characters may be entered in each field.

Street
Enter the street address for the customer in this text box. Up to 40 characters may be entered in this text field.

City, State, Zip
Enter the city, state and postal code information for the customer address in this text box. Up to 40 characters may be entered in this text box.

Comments Group

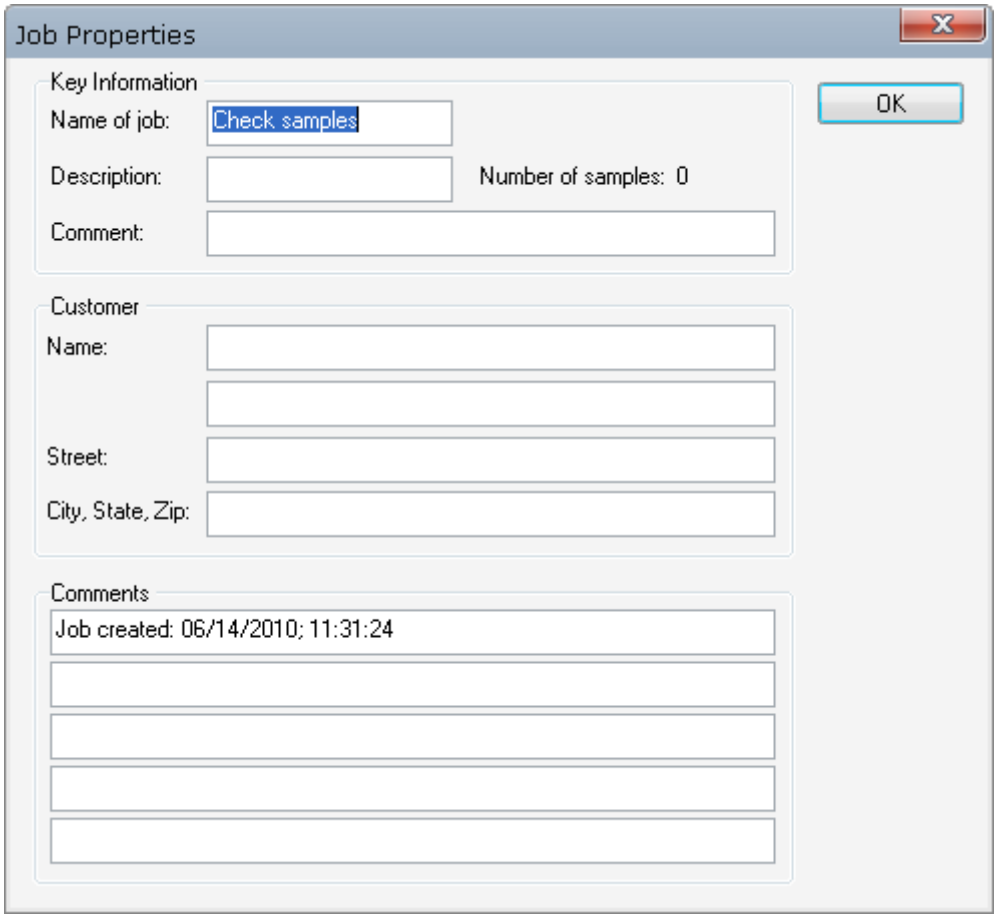
Enter comments about the job being created in these text boxes. Up to 80 characters may be entered in each of the text boxes.

After entering the new job´s data click on the *OK* command button to confirm the entries. The job will be created and automatically displayed in a new job window.

To cancel just click on the *Cancel* command button. Now, the job won´t be created.

1.4 Edit Job

Use this dialog to edit a job.



Key Information Group

Name of job
Edit the name of the job. The name may be up to 20 characters long and must be unique.

Description
Edit the description of the job. The description may be up to 20 characters long.

Customer Group

Name
Edit the customer's name and the name of the contact person, etc. as desired in these text boxes. Up to 40 characters may be entered in each field.

Street
Edit the street address for the customer in this text box. Up to 40 characters may be entered in this text field.

City, State, Zip
Edit the city, state and postal code information for the customer address in this text box. Up to 40 characters may be entered in this text box.

Comments Group

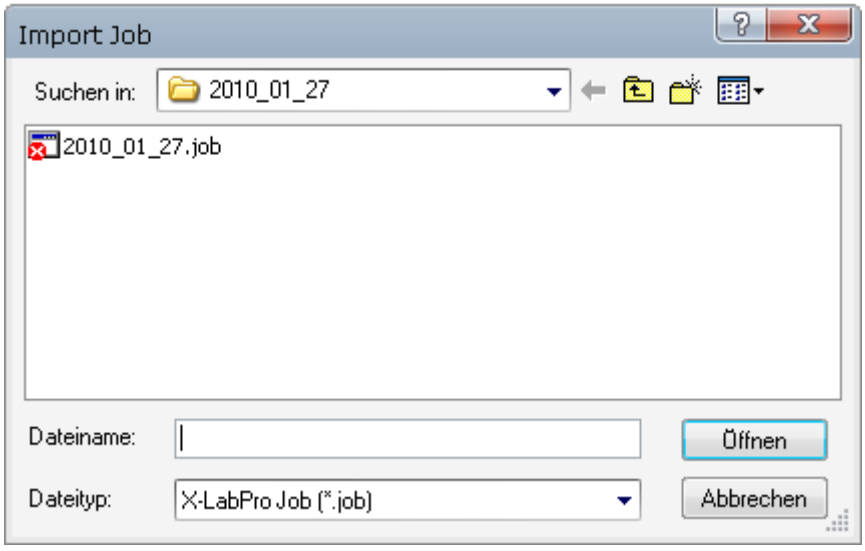
Edit the comments about the job in this text boxes. Up to 80 characters may be entered in each of the text boxes.

After editing the job´s data click on the *OK* command button to confirm the changes.

To cancel click on the *Cancel* command button and the job won´t be changed.

1.5 Import Job

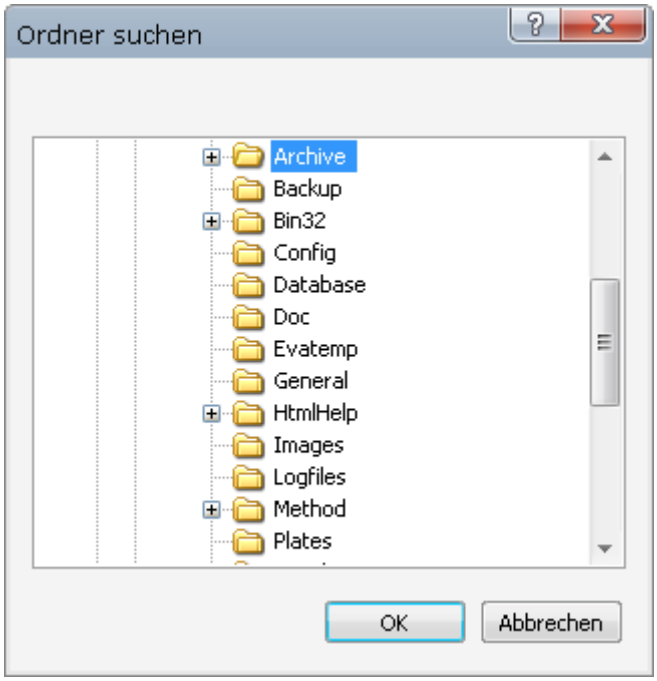
Use this dialog box to select the archive-file of the job you want to import.



For a detailed description how to import/export jobs please refer to the relevant chapter.

1.6 Export Job

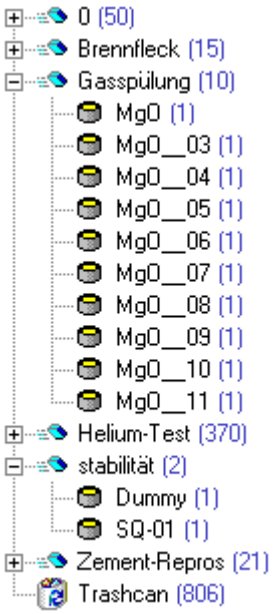
Use this dialog box to select the folder where you want to export a job.



For a detailed description how to import/export jobs please refer to the relevant chapter.

1.7 Tree Control

In the left area of the job manager it is possible to display the tree control.



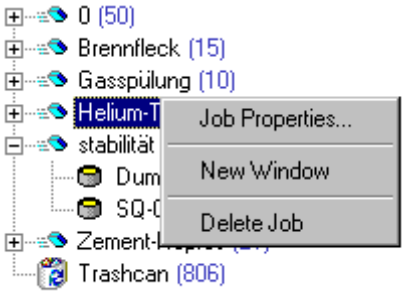
The tree control displays all the jobs and their assigned samples and measurements of the database. Further it displays the trashcan, where deleted samples are stored. To show or hide the tree control choose *Tree Control* of the

View menu (ALT, V, C). *Update* of the same menu will add valid database changes to the tree control.

Click on a job to display the assigned samples in the active job window. Double click on a job or sample item to fold open or back the children, clicking on a *plus* or *minus* icon of the tree is the same. The blue number maintain the numbers of children of the items.

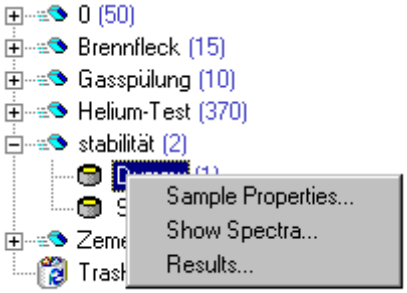
Right click on an item will give you access to a context menu in relation to the type (job, sample, measurement, trashcan).

1.8 Context Menu for a job



- **Job Properties**
  Select *Job Properties* to get the properties of the selected job. This selection opens the Job Properties dialog box.
- **New Window**
  Select *New Window* to open a new job window containing the selected job.
- **Delete Job**
  Select *Delete Job* to delete the selected job. This selection opens a dialog box to confirm the deletion. The assigned samples will be moved to the trashcan.

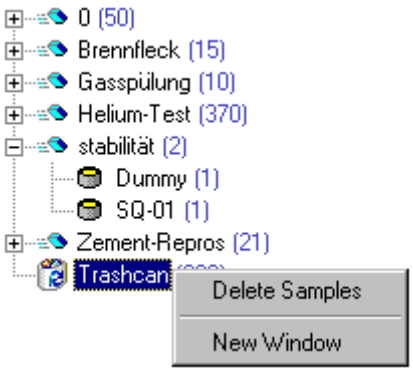
1.9 Context Menu for a sample



- **Sample Properties**
  Select *Sample Properties* to get the properties of the selected sample. This selection opens the Sample Properties dialog box.

- **Show Spectra**
  Select *Show Spectra* to open the X-LabPro Spectra Viewer and see the spectra of the selected sample.
- **Results**
  Select *Results* to get the results of the selected sample. This selection opens the Display Sample Results dialog box.

1.10 Context Menu for the trashcan



- **Delete All**
  Select *Delete All* to delete all samples in the trashcan.
- **New Window**
  Select *New Window* to open a new job window containing the trashcan.

Note: The job window offers you some more commands for the trashcan. For example, you can restore samples.

1.11 Menu Commands

1.11.1 Commands in the File Menu

- **Open Job**
  Use this command to open a job. This command opens a dialog box to select a job. The selected job will be opened in a new job window.
- **Shortcuts:**

  Toolbar:

  Keyboard: CTRL+O
- **Close Job**
  Use this command to close the active job window.

- **Shortcuts:**

  Keyboard: CTRL+Q

- **Print**
  Use this command to print the selected sample(s). This command opens a Print dialog box to do printer settings and the printing.

Shortcuts

Keyboard: CTRL+P

- **Print preview**
  Use this command to get a preview of the print-out on the screen.
- **Exit**
  Use this command to end your XLJobMan session. You can also use the *Close* command on the application control menu.

Shortcuts

Mouse: Double click the application's icon.
Keyboard: ALT+F4

1.11.2 Commands in the Edit Menu

- **New**
  Use this command to create a new sample. This command opens the Enter/Edit Sample Data dialog box to enter the new sample´s properties. If a sample is selected at the moment you use this command, the dialog box will be preset with the properties of the selected sample otherwise with defaults. The new sample will be assigned to the active job.
- **Edit**
  Use this command to edit the selected sample. This command opens the Enter/Edit Sample Data dialog box to change the sample´s properties.
- **Copy**
  Use this command to copy the selected sample(s) to the X-LabPro clipboard.

Shortcuts

Toolbar:
Keyboard: CTRL+C

- **Paste**
  Use this command to paste the sample(s) from the X-LabPro clipboard into the active job.

Shortcuts

Toolbar:
Keyboard: CTRL+V

- **Paste with Data**
  Use this command to paste the sample(s) including their results from the X-LabPro clipboard into the active job.

Shortcuts

Keyboard: CTRL+W

- **Clone**
  Use this command to clone the selected sample(s). The selected sample(s) will immediately be copied and pasted to the active job. The X-LabPro clipboard won´t be used.

Shortcuts

Toolbar:

Keyboard: CTRL+B

- **Delete**
  Use this command to delete the selected sample(s). The selected sample(s) will be moved to the trashcan.

Shortcuts

Toolbar:

Keyboard: CTRL+X

- **Assign Method**
  This command changes the method assignment of a sample.
- **Reset Measurements**
  This command resets the measurements of one or more selected samples.
- **Import Sample(s)**
  Use this command to import samples from archive-files (*.smp). This command opens a dialog box where you can select one or more files. The imported samples will be assigned to the active job.
- **Export Sample(s)**
  Use this command to export the selected samples to archive-files (*.smp). This command opens a dialog box where you can select the export folder.
- **Evaluate**
  Use this command to evaluate the selected sample(s)
- **Show Spectra**
  Use this command to open the X-LabPro Spectra Viewer to see the spectra of the selected sample(s).

Shortcuts

Toolbar:

- **Results**
  Use this command to get the results of the selected sample. This command opens the Display Sample Results dialog box.

Shortcuts

Toolbar:

- **Properties**
  Use this command to get the properties of the selected sample. This command opens the Sample Properties dialog box.

1.11.3 Commands in the View Menu

- **Toolbar**
  Use this command to display and hide the toolbar, which includes buttons for some of the most common commands in the Job Manager. A check mark appears next to the menu item when the toolbar is displayed.
  See Toolbar for help on using the toolbar.
- **Status Bar**
  Use this command to display and hide the status bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the status bar is displayed.
  See Status Bar for help on using the status bar.
- **Tree Control**
  Use this command to show and hide the tree control. The tree control shows the jobs and the assigned samples with measurements.
- **Update**
  Use this command to update the tree control after valid database changes have been made from X-LabPro. When using this command the tree will only be reloaded from its temporary files.
- **Rebuild**
  Use this command to update the tree control after valid database changes have been made from X-LabPro. When using this command the tree will completely re-calculated from the database. This operation will take a few seconds.

1.11.4 Commands in the Window Menu

The *Window* menu contains the following commands.

- **New Window**
  Select this menupoint to open a new job window.
- **Cascade**
  Select this menupoint to arrange open windows so that the title bar of each window is visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.

- **Tile**
  Select this menupoint to arrange all of the open windows side by side so that all of them are visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.
- **Arrange Icons**
  Select this menupoint to arrange the icons within the application window.

1.11.5 Commands in the X-LabPro Menu

The *X-LabPro* menu contains the following commands to open other applications:

- **Method Administration...**
  Use this command to open the Method Administration. You may also click on the button on the toolbar.
- **Job Manager...**
  This command would open the Job Manager. It is disabled because the Job Manage is already running.
- **Routine Dialog...**
  Use this command to open the Routine Dialog. You may also click on the button on the toolbar.
- **Spectra Viewer...**
  Use this command to open the Spectra Viewer. You may also click on the button on the toolbar.
- **Configuration Editor...**
  Use this command to open the Configuration Editor.
- **Evaluation...**
  Use this command to open the Evaluation Tool.

1.11.6 Commands in the Help Menu

The *Help* menu contains the following commands which will assist you by using this application:

- **Contents**
  Select this menupoint to display a table of contents for the help system of the X-LabPro applications. In the help system, select the *Contents* command button below the menuline to show the table of contents.
- **Context Sensitive**
  Select this menupoint to display a context sensitive help text. This menupoint corresponds to the command button with a question mark in the toolbar.
- **Software**
  Select this menupoint to display a table of contents for the software description. Use of the operation and control software for the X-LAB energy dispersive x-ray fluorescence spectrometer is described in this section.

- **Shortcuts**
  Select this menupoint to display an overview of the keyboard shortcuts.
- **About XLJobMan**
  Show the version and copyrights of the Job Manager.

1.12 Other

1.12.1 Toolbar

The toolbar is displayed across the top of the application window, below the menu bar. It provides quick mouse access to many functions used in the job manager. To hide or display the toolbar, choose *Toolbar* from the *View* menu (ALT, V, T).

Click to

	Create a new job and open it in a new job window.
	Open a dialog to select a job. The selected job will be opened in a new job window.
	Copy the selected sample(s) to the X-LabPro clipboard.
	Paste the sample(s) in the X-LabPro clipboard to the active job.
	Clone the selected sample(s). The selected sample(s) will immediately be copied and pasted to the active job. The clipboard will not be used for this operation.
	Delete the selected sample(s). The selected sample(s) will be moved to the trashcan.
	Open the X-LabPro Spectra Viewer to show the spectra of the selected sample(s).
	Open the Display Sample Results dialog box to show the results of the selected sample.
	Print the selected sample(s).
	Open the Online Help.
	Open the Method Administration.This button is disabled because the Method Administration is already running.
	Open the Job Manager.
	Open the Routine Dialog.
	Open the Spectra Viewer.

1.12.2 Title Bar

The title bar is located along the top of the application window. It contains the names of the application and of the current job window.

To move the window, drag the title bar. *Note*: You can also move dialog boxes by dragging their title bars.

The title bar may contain the following elements:

	Exit button
	Maximize button
	Minimize button
	Name of the application
	Name of the job window
	Icon of the application

1.12.3 Status Bar

The status bar is displayed at the bottom of the Job Manager. To display or hide the status bar, use the *Status Bar* command in the *View* menu.

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area shows messages that describe the action of a toolbar button while pressing the button. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button.

Moreover the database reading status will be shown in the status bar by a progress bar.

The right areas of the status bar indicate which of the following keys are latched down:

Indicator Description

CAP	The Caps Lock key is latched down.
NUM	The Num Lock key is latched down.
SCRL	The Scroll Lock key is latched down.

2 Routine Dialog

The Routine Dialog offers the user an easy use of the X-Lab^{Pro} routine measurement.

It is possible to enter the sample data in the right area of the screen, the sample table. The left area contains a tab control for the selection of different view modes during the measurement. It is possible to switch between the

- Sample Plate Display
- Spectrum Display
- Video Display (if your instrument is equipped with a video camera system).
- Comunication
- Element Mapping (MIDEX equipped with xyz stages only)

The following menus are displayed when the Routine window is active:

- File Menu
- Edit Menu
- View Menu
- Tools Menu
- Recalibration Menu
- Video Menu
- Help Menu
- System Menu

See also:

Toolbar
Statusbar

2.1 The X-LabPro Routine Dialog

The Routine Dialog offers the user an easy use of the X-Lab^{Pro} routine measurement.

It is possible to enter the sample data in the right area of the screen, the sample table. The left area contains a tab control for the selection of different view modes during the measurement. It is possible to switch between the

- Sample Plate Display
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- Element Mapping (MIDEX equipped with xyz stages only)

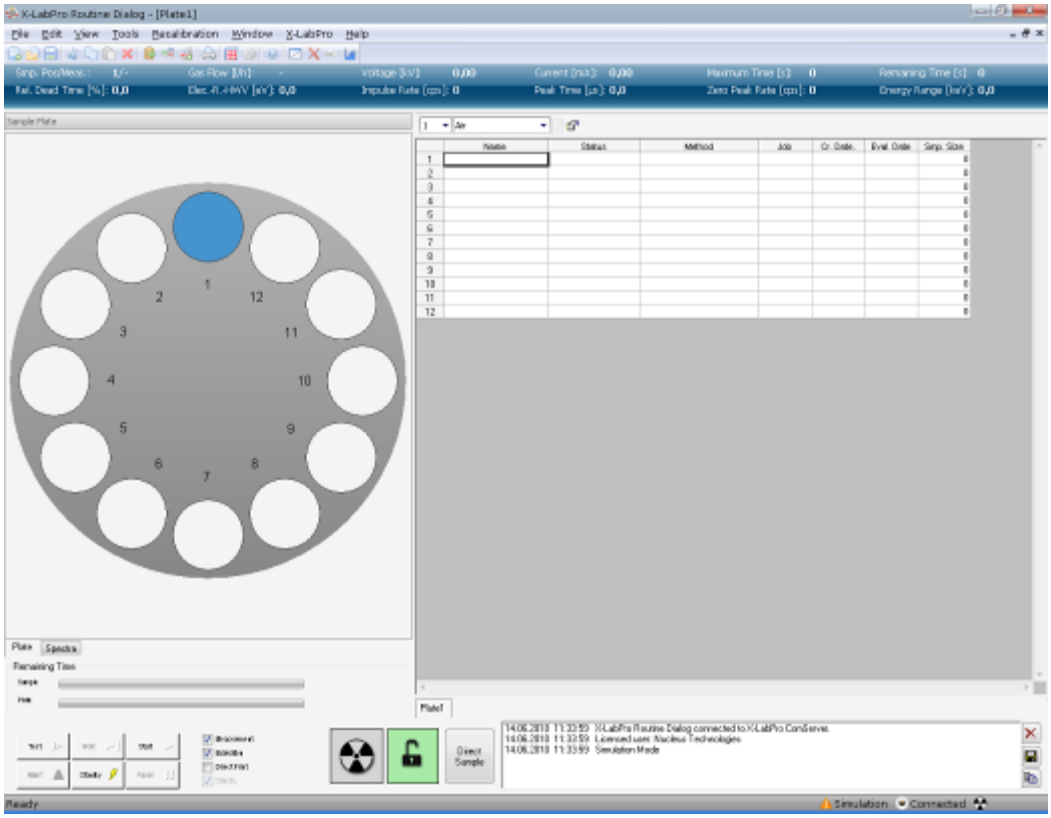
The following menus are displayed when the Routine window is active:

- File Menu
- Edit Menu
- View Menu
- Tools Menu
- Recalibration Menu
- Video Menu
- Help Menu
- System Menu

See also:

Toolbar
Statusbar

2.2 How to Define New Samples/Enter the Sample Data (Xepos)



By clicking a cell in the "Name" column this will be highlighted and you can enter the sample name using the keyboard. After leaving this cell by pressing the "Enter" key, an arrow key or clicking into another cell, the sample name is accepted.

Moreover, the job name will generated automatically as configurated. You can overwrite the job name if necessary.

Use the mouse to select a method from the method field. By clicking on the method field, a drop down list opens and it is possible to select a method. Only the methods of the selected method class will be displayed in the drop down list.

For editing additional sample data it is possible to display the respective columns by changing the configuration in the Routine Dialog Settings Dialog Box in the Configuration Editor. For changing additional data without displaying the columns, click with the right mouse button on the respective cell containing the sample name and select the Sample Data menu point from the context menu. The Enter/Edit Sample Data Dialog Box opens.

It is possible to select another method class for your sample plate by using the drop down list box above the sample table. In the example the method class "Vac methods" is in use.
Note: By selecting a new method class all contents of the sample table will be deleted.

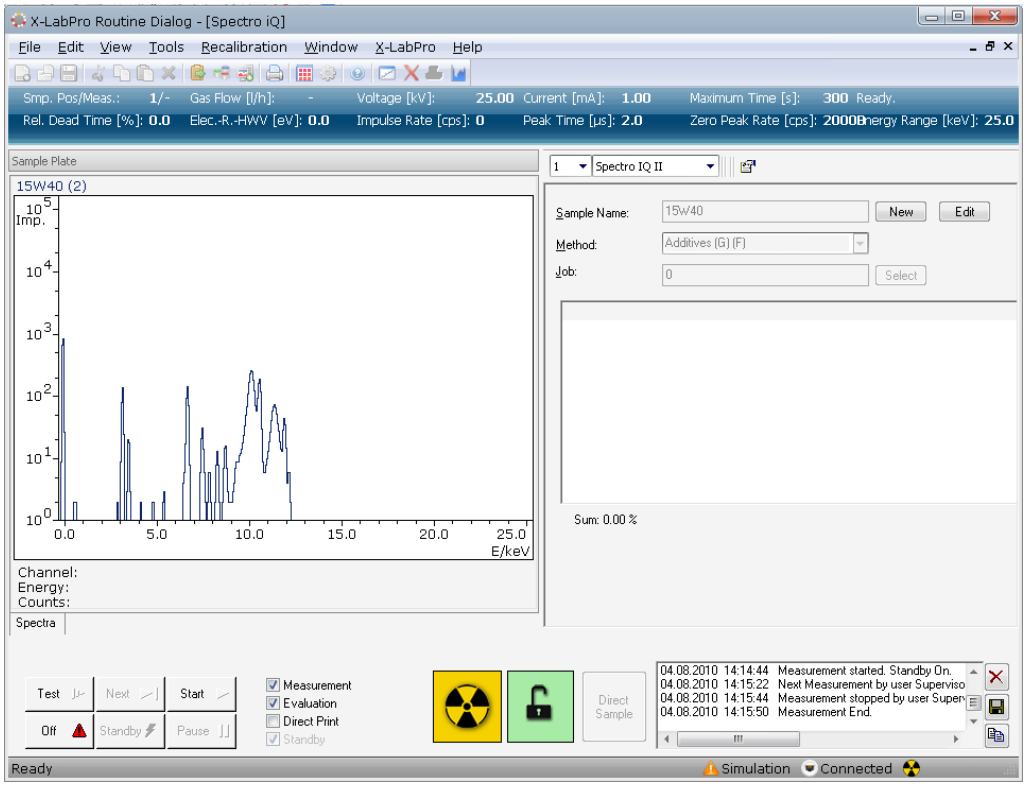
It is possible to define the sample plate for repeated runs by selecting a repetition number from the drop down list box left above the sample table (Here only 1 run is selected).

You can use the following shortcuts to use the clipboard:

- Use the "Del" key to delete the content of the selected field or the whole sample, if the belonging row is selected in the table.
- Use "Ctrl+Ins" or "Ctrl+C" to copy selected table areas into the clipboard.
- Use "Shift+Ins" or "Ctrl+V" to paste the data from the clipboard into the selected table area.
- Use "Shift+Del" or "Ctrl+X" to cut selected table areas into the clipboard.

You can edit the entered data at every time before the measurement is started. Just click into the cell to overwrite the contained data.

2.3 How to Define New Samples/Enter the Sample Data (IQ)



By clicking in the "Sample Name" edit box you can enter the sample name using the keyboard. Moreover, the job name will generated automatically as configurated. You can overwrite the job name if necessary.

Use the mouse to select a method from the "Method" drop down list. Only the methods of the selected method class will be displayed in the drop down list.

For editing additional sample data click with the right mouse button in the "Sample Name" edit box and select the Sample Data menu point from the context menu. The Enter/Edit Sample Data Dialog Box opens.

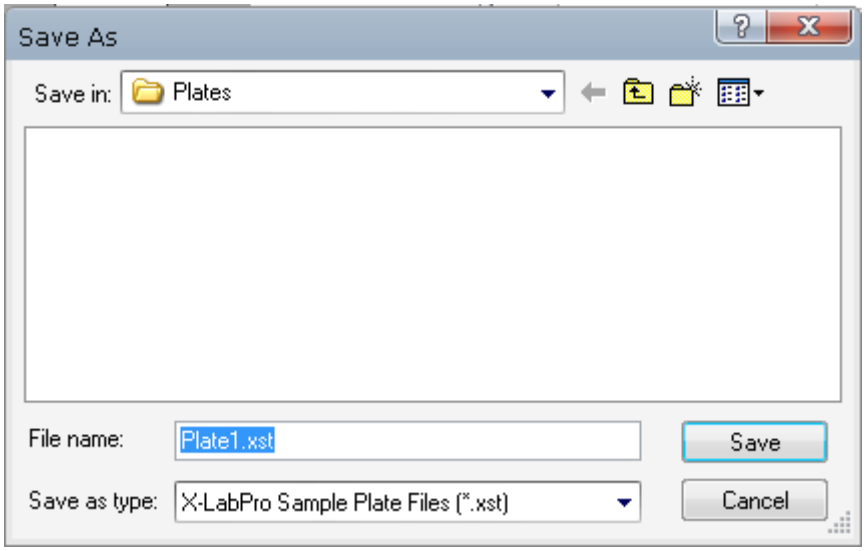
It is possible to select another method class by using the drop down list box above the "Sample Name" edit box. In the example the method class "SPECTRO IQ" is in use.

It is possible to define a sample measurement for repeated runs by selecting a repetition number from the drop down list box left above the sample table (Here only 1 run is selected).

You can edit the entered data at every time before the measurement is started.

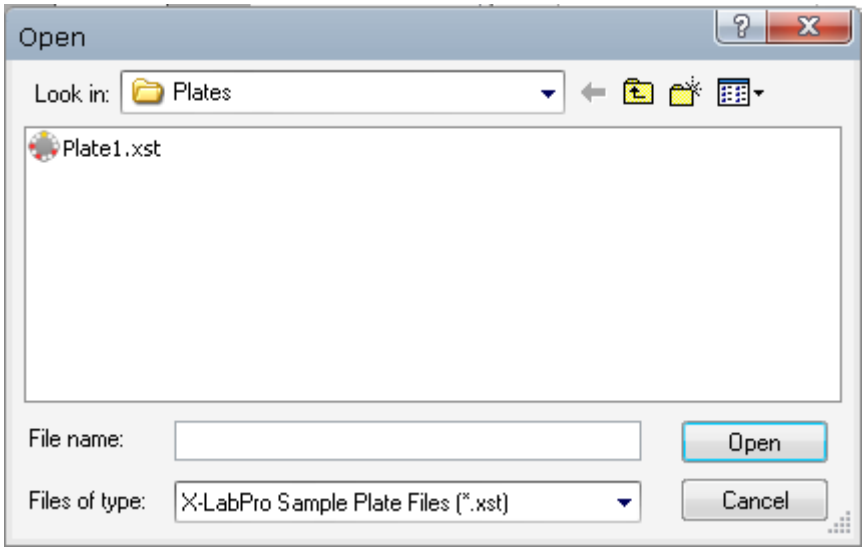
2.4 How to Load and Save the Sample Plates

At every time it is possible to save the entered sample data for later use. To do this use the menu point *Save as* of the *File Menu*. The *Save As dialog box* opens like shown in the picture below:



Enter a file name for your sample plate. By clicking the "Save" command button the sample plate data will be saved. The file type is "xst" ("***X***-Lab[Pro] ***S***ample ***T***able").

To open a saved sample plate later, use the *File Open* command in the *File Menu*. The *File Open dialog* shown in the picture below will open and you can select one of the files shown in the dialog box.



2.5 The Measurement

After entering all sample plate data or loading a sample plate, the measurement can be started by clicking the *Start* button shown below. The following picture shows the control panel of the Routine Dialog.

For an IQ you have to enter a sample name in the Sample Name Eedit field. The following picture shows the control panel of the Routine Dialog if your intrument is a IQ.

The command buttons have the following functions:

- Start – Starts the measurement. Will be switched during the measruement to
- Stop – Measurement will be stopped (Standby Mode will be entered if selected)
- Abort – Measurement will be stopped (Standby Mode will not be entered)
- Pause – Measurement will be paused. Continue by clicking *Start*
- Test – Starts a test measurement after entering all measurements parameters

- Next – During the measurement: The current measurement will be breaked and the next measurement will be started
- Standby – The standby mode of the instrument can be switched on or off
- Reset – The actually measurement will be restarted
- Off – Turn off the instrument (IQ only)

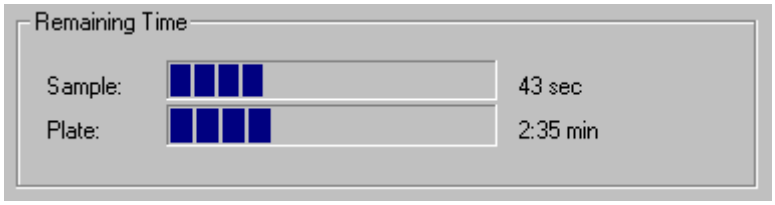
The check boxes on the right have the following functions:

- Measurement – The samples of the current selected sample plate will be measured
- Evaluation – The samples of the current selected sample plate will be evaluated
- Direct Print – The sample results will be printed directly after the measurement is done
- Standby – After the measurement is completed the instrument will be switched into the standby mode.

After the measurement is started the samples will be shown in different colors. The colors have the following symbols (Xepos only):

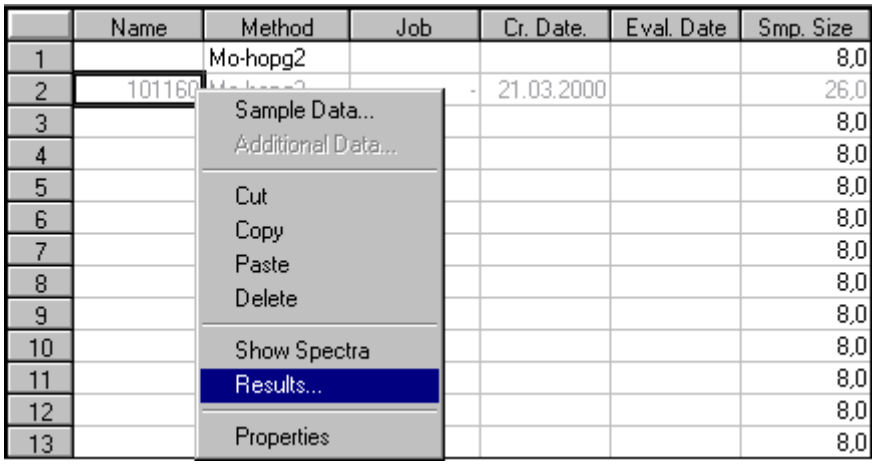
- Red = The sample is not measured completely
- Yellow = This sample is in measurement
- Green = The sample is measured completely

The remaining time will be displayed like in the following picture (Xepos only):

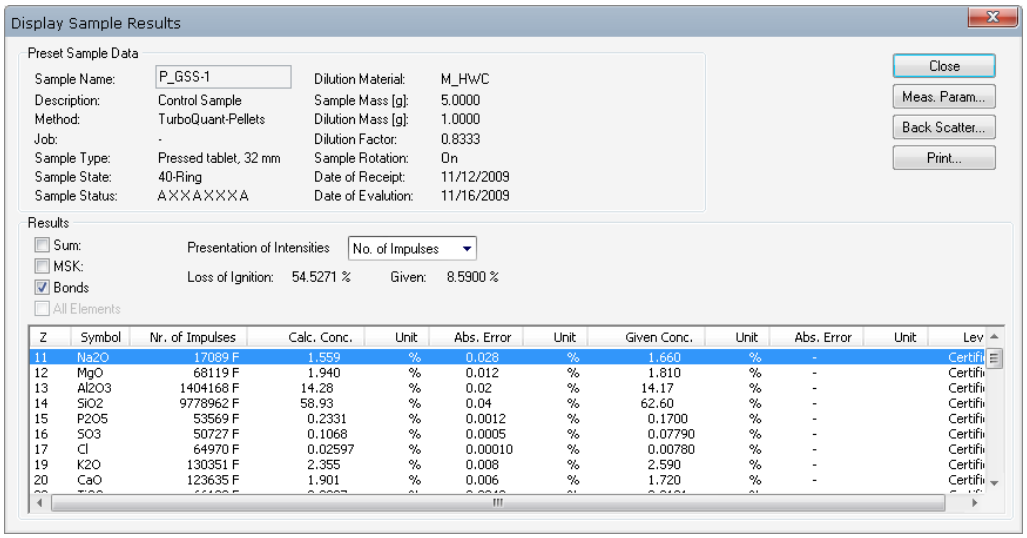


2.6 Show the Sample Results

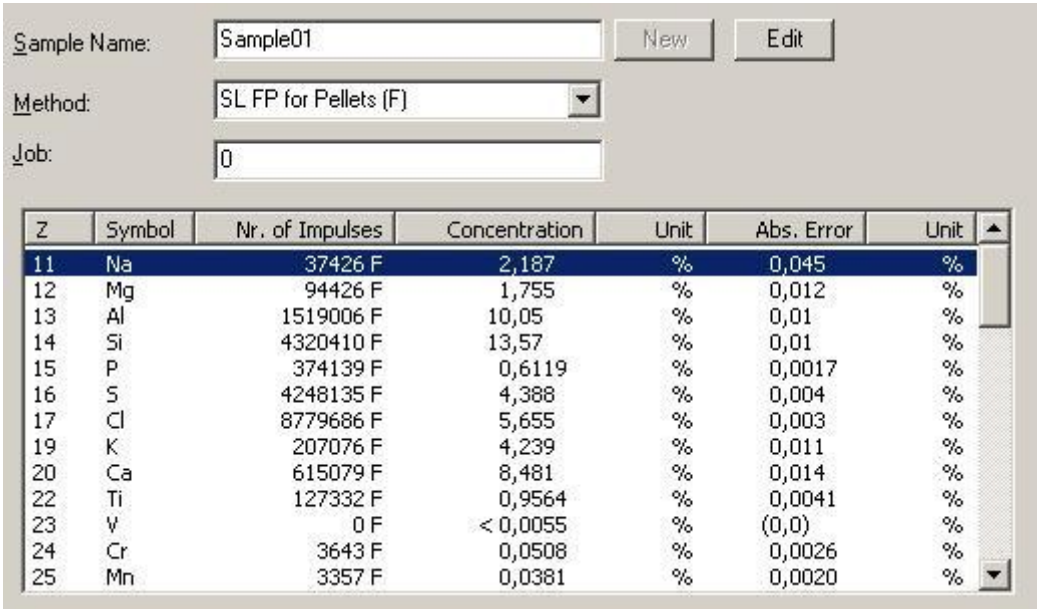
After the measurement and evaluation of a sample is finished, you can open the context menu by clicking the right mouse button on the sample name. The context menu is shown in the following picture:



Select the *Results* menu point to open the *Display Sample Results Dialog Box:*


Display Sample Results
Preset Sample Data
Sample Name: P_GSS-1
Description: Control Sample
Method: TurboQuant-Pellets
Job: -
Sample Type: Pressed tablet, 32 mm
Sample State: 40-Ring
Sample Status: AXXAXXXA
Dilution Material: M_HWC
Sample Mass [g]: 5.0000
Dilution Mass [g]: 1.0000
Dilution Factor: 0.8333
Sample Rotation: On
Date of Receipt: 11/12/2009
Date of Evalution: 11/16/2009
Close
Meas. Param...
Back Scatter...
Print...
Results
Sum:
MSK:
Bonds
All Elements
Presentation of Intensities
No. of Impulses
Loss of Ignition: 54.5271 %
Given: 8.5900 %
Z Symbol Nr. of Impulses Calc. Conc. Unit Abs. Error Unit Given Conc. Unit Abs. Error Unit Lev
11 Na2O 17089 F 1.559 % 0.028 % 1.660 % - Certifi
12 MgO 68119 F 1.940 % 0.012 % 1.810 % - Certifi
13 Al2O3 1404168 F 14.28 % 0.02 % 14.17 % - Certifi
14 SiO2 9778962 F 58.93 % 0.04 % 62.60 % - Certifi
15 P2O5 53569 F 0.2331 % 0.0012 % 0.1700 % - Certifi
16 SO3 50727 F 0.1068 % 0.0005 % 0.07790 % - Certifi
17 Cl 64970 F 0.02597 % 0.00010 % 0.00780 % - Certifi
19 K2O 130351 F 2.355 % 0.008 % 2.590 % - Certifi
20 CaO 123635 F 1.901 % 0.006 % 1.720 % - Certifi

For a IQ the sample results will be shown automatically after the measurement and evaluation of a sample is finished.

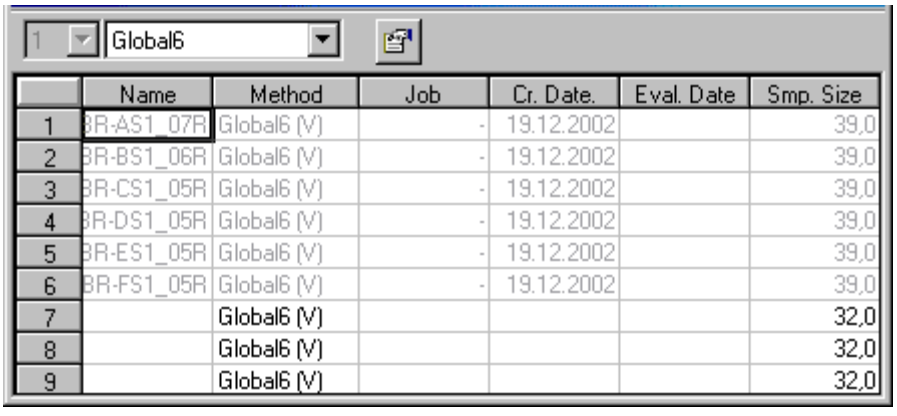


Z	Symbol	Nr. of Impulses	Concentration	Unit	Abs. Error	Unit
11	Na	37426 F	2,187	%	0,045	%
12	Mg	94426 F	1,755	%	0,012	%
13	Al	1519006 F	10,05	%	0,01	%
14	Si	4320410 F	13,57	%	0,01	%
15	P	374139 F	0,6119	%	0,0017	%
16	S	4248135 F	4,388	%	0,004	%
17	Cl	8779686 F	5,655	%	0,003	%
19	K	207076 F	4,239	%	0,011	%
20	Ca	615079 F	8,481	%	0,014	%
22	Ti	127332 F	0,9564	%	0,0041	%
23	V	0 F	< 0,0055	%	(0,0)	%
24	Cr	3643 F	0,0508	%	0,0026	%
25	Mn	3357 F	0,0381	%	0,0020	%

2.7 Prepare Global Recalibration

If a global recalibration is necessary, use the menu point *Prepare Global Recalibration* of the *Recalibration* menu. Remember that reference samples defined once in X-LabPro are required for a propper work of this function.

The routine dialog itself will create a new global sample plate like shown in the following picture:



	Name	Method	Job	Cr. Date.	Eval. Date	Smp. Size
1	BR-AS1_07R	Global6 (V)	-	19.12.2002		39,0
2	BR-BS1_06R	Global6 (V)	-	19.12.2002		39,0
3	BR-CS1_05R	Global6 (V)	-	19.12.2002		39,0
4	BR-DS1_05R	Global6 (V)	-	19.12.2002		39,0
5	BR-ES1_05R	Global6 (V)	-	19.12.2002		39,0
6	BR-FS1_05R	Global6 (V)	-	19.12.2002		39,0
7		Global6 (V)				32,0
8		Global6 (V)				32,0
9		Global6 (V)				32,0

The routine dialog for an IQ will also create a new global sample like shown in the following picture:

New recalibration samples with a continuous numbered sample name (e.g. "_07R", "_06R",...) will automatically be generated as defined in the configuration editor. These samples will automatically contain a link to the original reference sample as control sample.

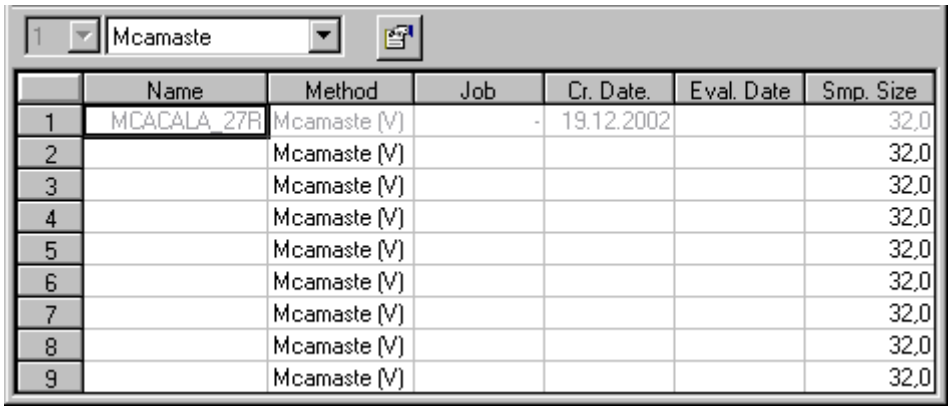
Use this function only to prepare and start a global recalibration.

Do not try to edit the automatically generated sample plate manually.

2.8 Prepare MCA Recalibration

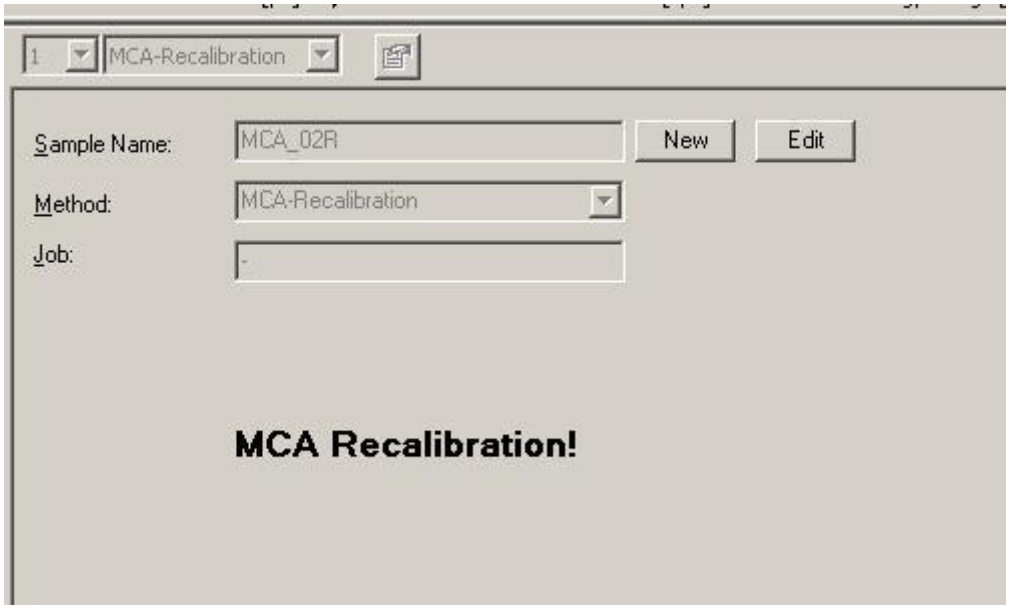
If an MCA recalibration is necessary, use the menu point *Prepare MCA Recalibration* of the *Recalibration* menu. Remember that a reference sample defined once in X-LabPro is required for a propper work of this function.

The routine dialog itself will create a new MCA sample plate like shown in the following picture:



	Name	Method	Job	Cr. Date.	Eval. Date	Smp. Size
1	MCACALA_27R	Mcamaste (V)	-	19.12.2002		32,0
2		Mcamaste (V)				32,0
3		Mcamaste (V)				32,0
4		Mcamaste (V)				32,0
5		Mcamaste (V)				32,0
6		Mcamaste (V)				32,0
7		Mcamaste (V)				32,0
8		Mcamaste (V)				32,0
9		Mcamaste (V)				32,0

The routine dialog for an IQ will also create a new MCA sample like shown in the following picture:



New MCA samples with a continous numbered sample name (e.g. "_27R", "_28R",...) will automatically be generated as defined in the configuration editor. These samples will automatically contain a link to the original reference sample as control sample.

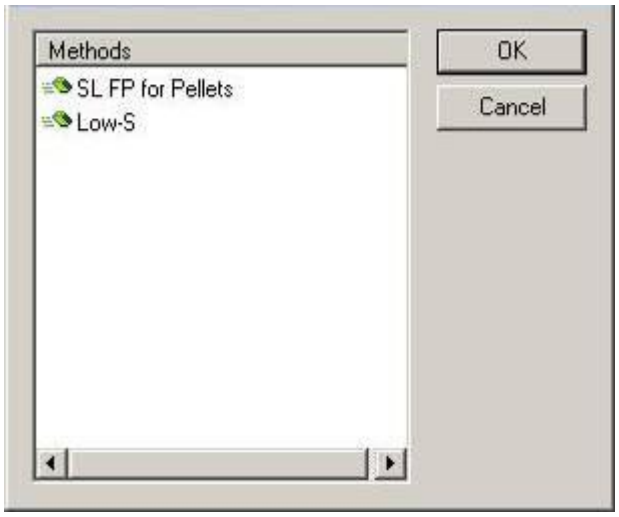
Use this function only to prepare and start an MCA recalibration.

Do not try to edit the automatically generated sample plate manually.

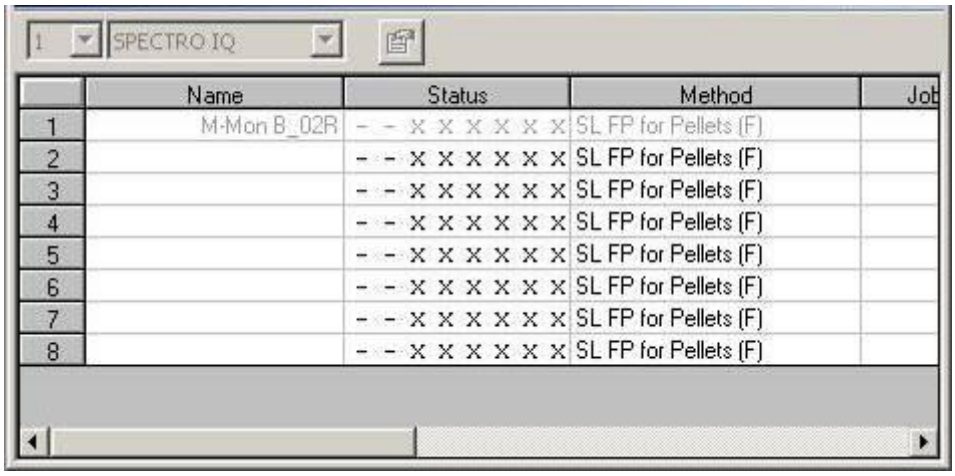
2.9 Prepare Intercept Recalibration

If an Intercept recalibration is necessary, use the menu point *Prepare Intercept Recalibration* of the *Recalibration* menu. A dialog box for method selection will be opened. Select the method that should be calibrated in this dialog box.

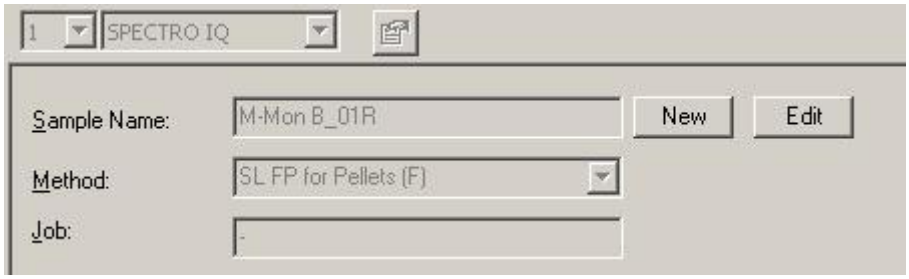
Remember that a reference sample defined once in Method Administration is required for a propper work of this function.



The routine dialog itself will create a new Intercept sample plate like shown in the following picture:


1
SPECTRO IQ
Name
Status
Method
Job
1 M-Mon B_02R - - X X X X X X SL FP for Pellets (F)
2 - - X X X X X X SL FP for Pellets (F)
3 - - X X X X X X SL FP for Pellets (F)
4 - - X X X X X X SL FP for Pellets (F)
5 - - X X X X X X SL FP for Pellets (F)
6 - - X X X X X X SL FP for Pellets (F)
7 - - X X X X X X SL FP for Pellets (F)
8 - - X X X X X X SL FP for Pellets (F)

For an IQ the routine dialog look like the following picture:



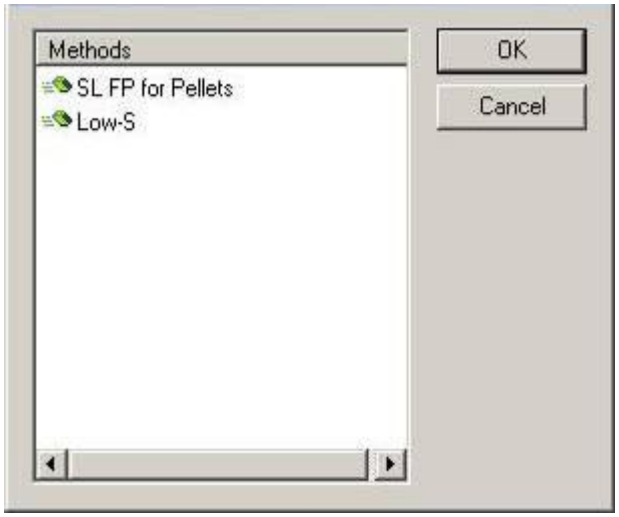
New Intercept samples with a continous numbered sample name (e.g. "_27R", "_28R",...) will automatically be generated as defined in the configuration editor. These samples will automatically contain a link to the original reference sample as control sample.

Use this function only to prepare and start an Intercept recalibration.

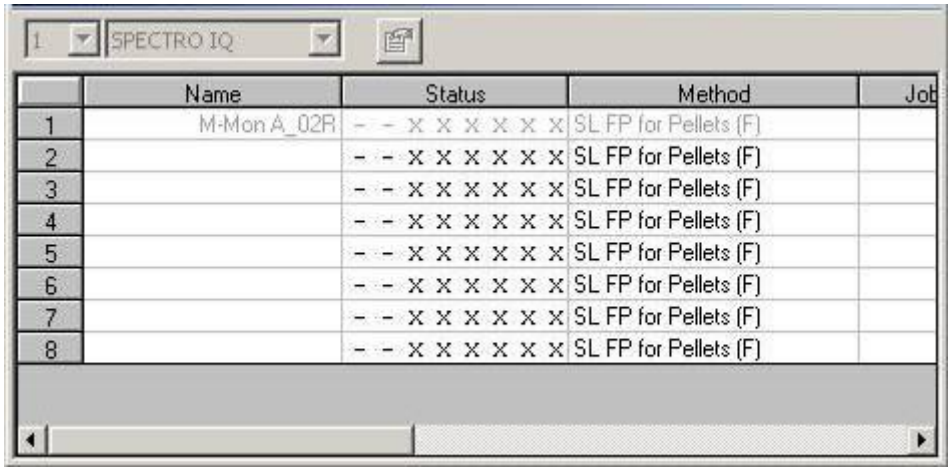
2.10 Prepare Method Recalibration

If an Method recalibration is necessary, use the menu point *Prepare Method Recalibration* of the *Recalibration* menu. A dialog box for the method selection will be opened. Select in this dialog box the method that should be calibrated

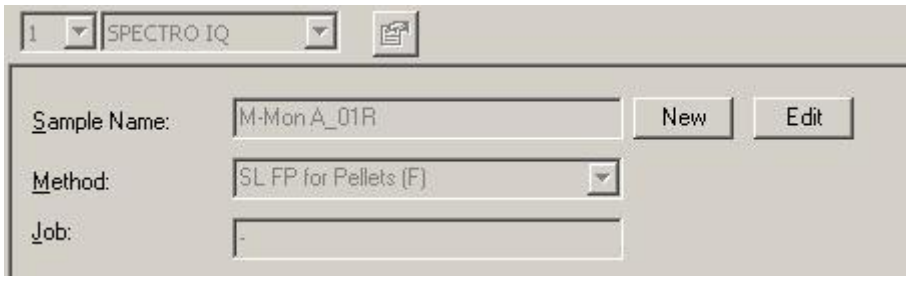
Remember that a reference sample defined once in Method the Administration is required for a propper work of this function.



The routine dialog itself will create a new Method sample plate like shown in the following picture:


1
SPECTRO IQ
Name
Status
Method
Job
1 M-Mon A_02R - - X X X X X X SL FP for Pellets (F)
2 - - X X X X X X SL FP for Pellets (F)
3 - - X X X X X X SL FP for Pellets (F)
4 - - X X X X X X SL FP for Pellets (F)
5 - - X X X X X X SL FP for Pellets (F)
6 - - X X X X X X SL FP for Pellets (F)
7 - - X X X X X X SL FP for Pellets (F)
8 - - X X X X X X SL FP for Pellets (F)

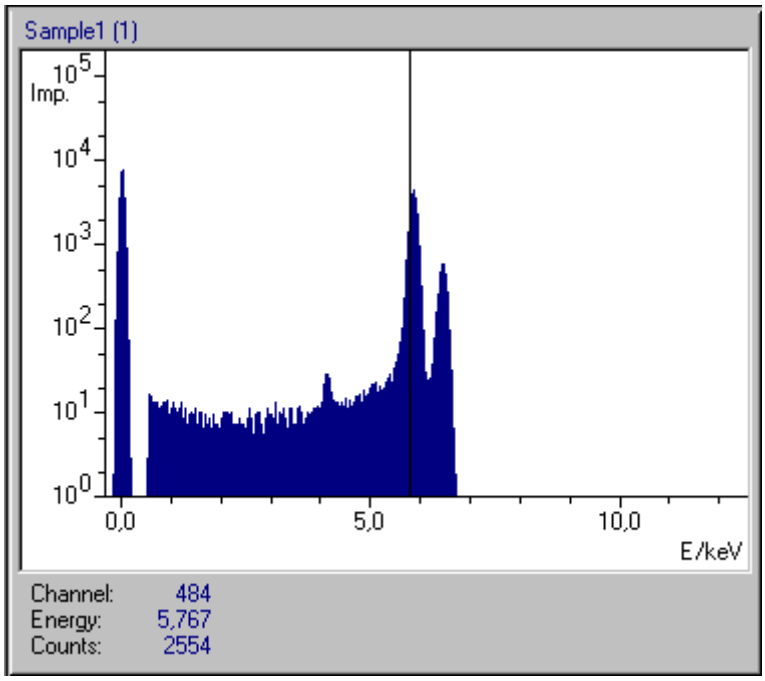
For an IQ the routine dialog look like the following picture:



New Mehod samples with a continous numbered sample name (e.g. "_27R", "_28R",...) will automatically be generated as defined in the configuration editor. These samples will automatically contain a link to the original reference sample as control sample.

Use this function only to prepare and start an Method recalibration.

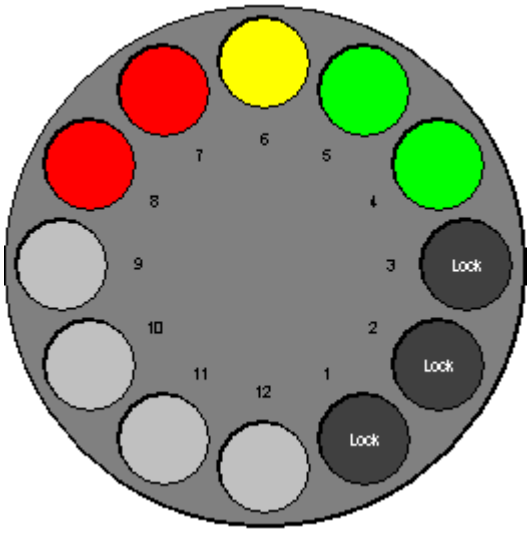
2.11 The Routine Dialog Spectrum Display



The spectrum display shows the spectrum that is transmitted from the instrument. On the top the sample name of the current measured sample and the measurement number is displayed.
On the bottom the line cursor data for the current line cursor position is displayed. Click into the spectrum display to place the line cursor.

Use the Toolbox to have enhanced access to the spectral representation. You can open the toolbox by using the Toolbar symbol or the Tools Menu.

2.12 The Routine Dialog Sample Plate Display



The sample plate display can be selected by using the tab control in the middle left of the Routine Dialog screen. It shows the instrument sample plate status at its current situation.

The different colors have the following significance:

Dark Gray (with text "Lock")
Locked Position. You cannot place samples on this plate position. Locked positions can be defined in the Configuration Editor by using the Routine Dialog Settings Dialog Box.

Green
Measurement of this sample is completed

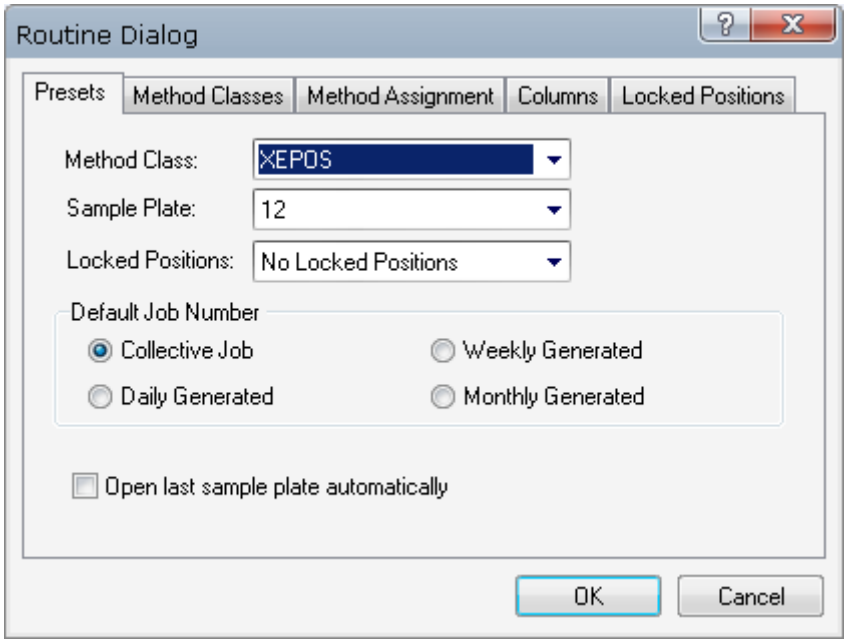
Yellow
Measurement of this sample in progress

Red
Measurement of this sample is not completed

Blue (during editing the sample table)
This position is selcted for entering sample data

2.13 Settings Dialog Box

The presets for the Routine Dialog can be configured using the Configuration Editor. Click with the right mouse button on the X-LabPro communication server (small icon in the tray, left to the clock) and click *Configuration Editor*. After double-clicking the *Routine Dialog* icon, the following dialog opens:



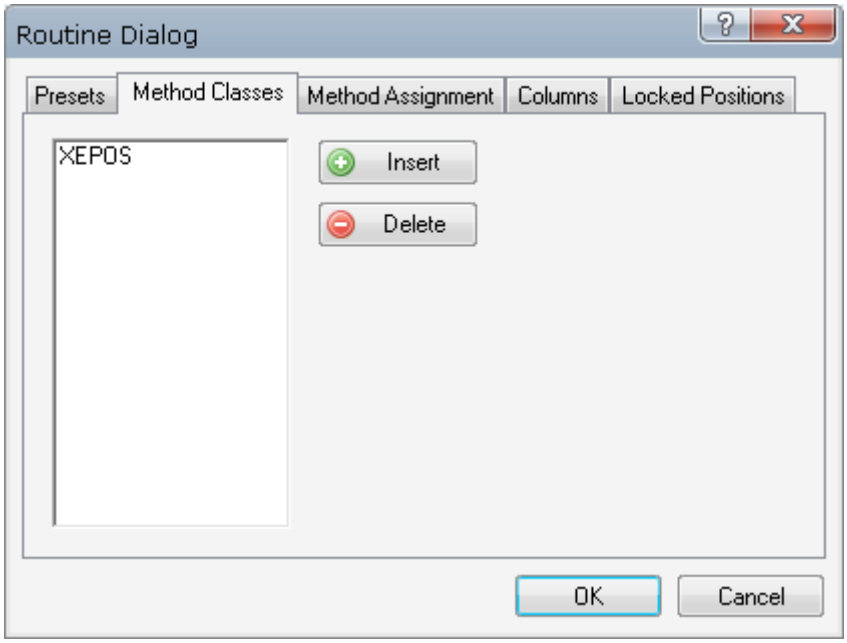
Here the method class, a sample plate and a list of locked positions can be selected as pre-setted for the Routine Dialog. Moreover you can decide how the job name will be created automatically. You can choose between collective job as automatically used, a daily generated job (e.g. 2001_06_05), a weekly generated job (e.g. 2001_23) or a monthly generated job (e.g. 2001_06).

Note: A job can include a maximum of 1000 samples.

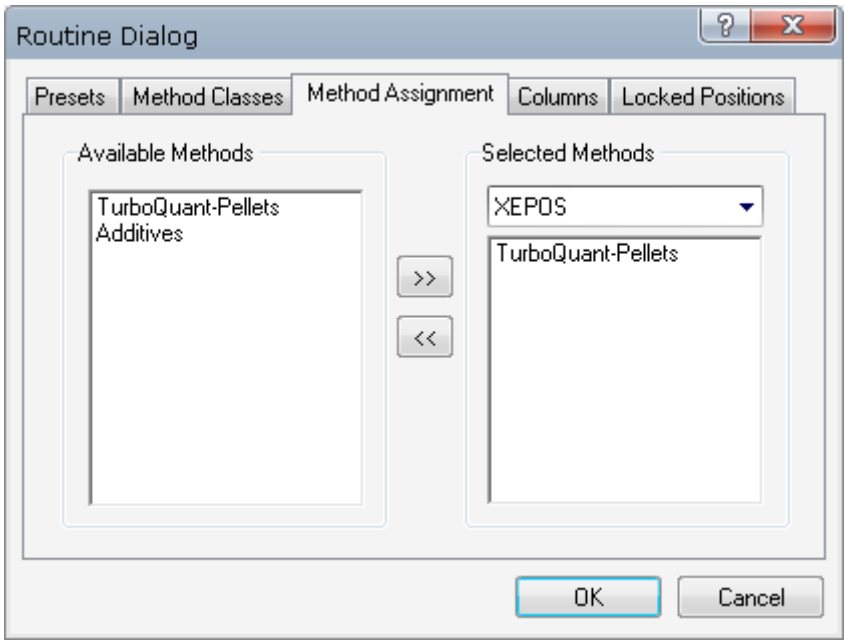
If you measure a lot of samples it will be useful to use weekly or daily generated jobs.

The check box at the bottom of the dialog can be used to start the Routine Dialog automatically with X-LabPro.

You must define at least one method class. Click on the *Method Class* tab control to open the following sheet:



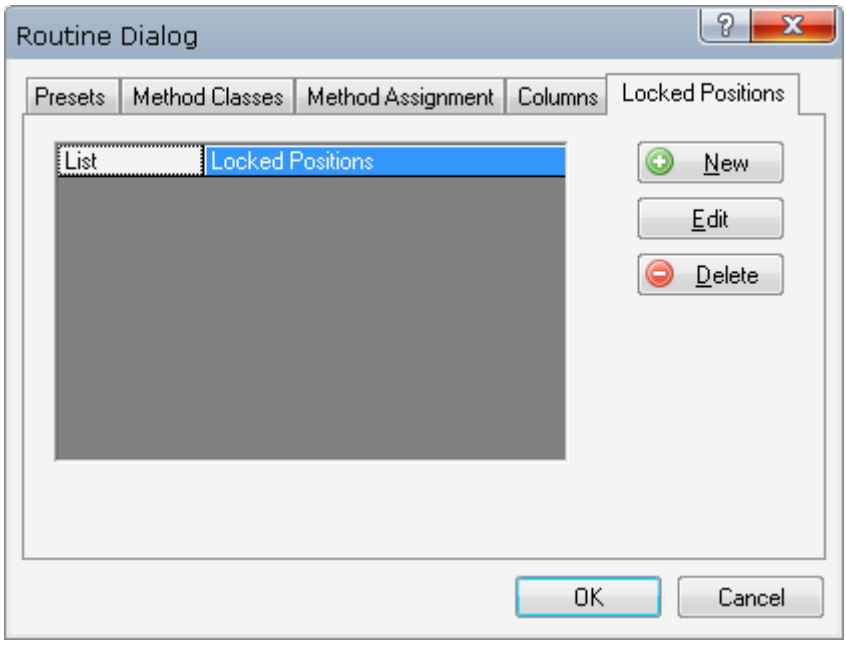
The picture shows a system containing 3 method classes. Up to 20 method classes can be defined. Use the *Insert* and *Delete* button to manage your method classes. After you have defined the method classes use the *Method Assignment* sheet to assign the methods to the defined classes.



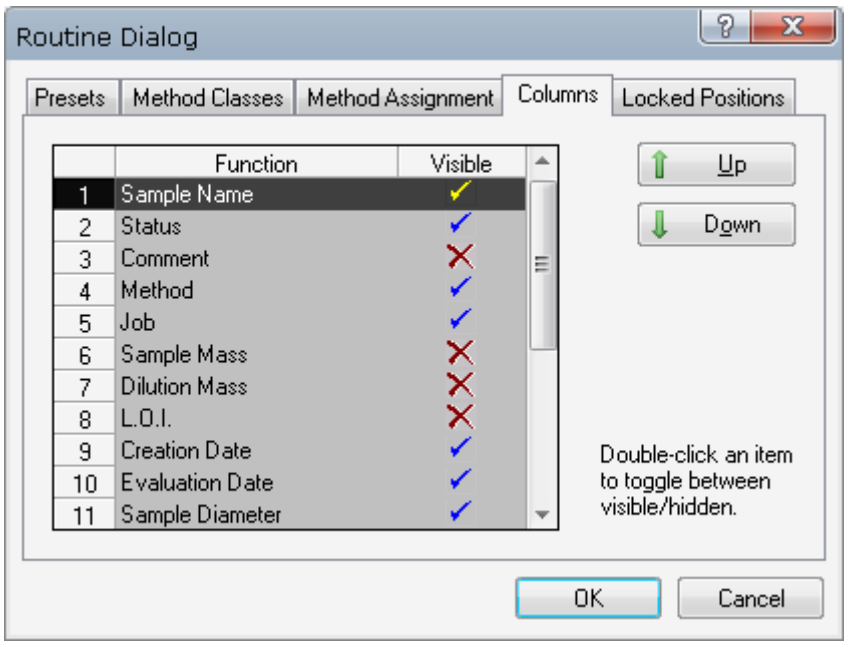
Select the method class in the drop down list at the top right of the dialog. Use *Insert* to add selected methods from the list at the left to the selected method class represented by the right list. Use *Delete* to remove a selected method from the right list.

Click to the *Locked Positions* sheet to define the list of locked positions as shown in the picture below. Use *New* to open the *Edit Locked Positions* dialog box for

selecting locked positions. By clicking *Edit* you can edit the selected list of locked positions. Click *Delete* for deleting the selected list of locked positions.



In the *Columns* sheet you can define the order of the columns and select if you want the columns to be visible or hidden. Use the *Up* and *Down* buttons to change the order position of a selected column. Double-click on a column to change between visible or hidden.



After the configuration is finished it is meaningful to edit and check the settings on the first sheet *Presets* again and to save the configuration. Restart all the X-LabPro applications to make user of the new settings.

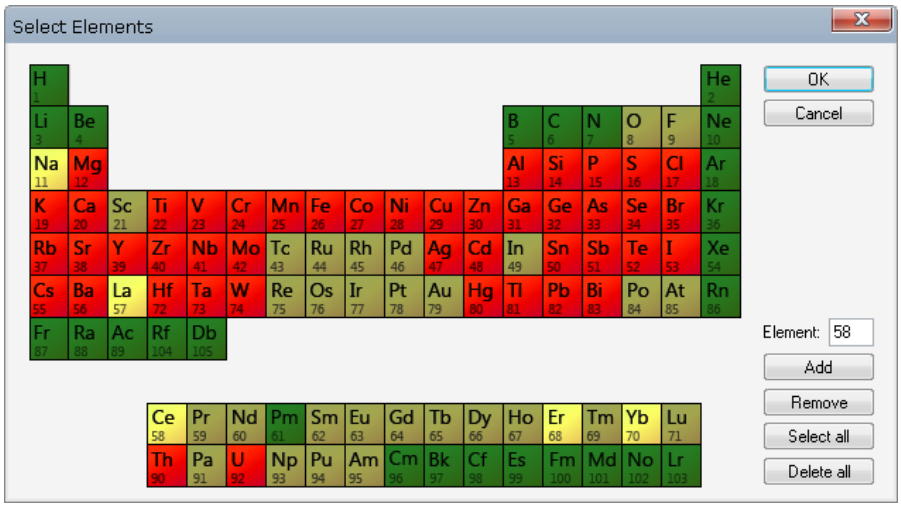
If you want to change the settings for a selected plate in the Routine Dialog, use the *Settings* dialog box that can be opened by clicking *Settings* in the *Extras* menu.

3 Result Viewer

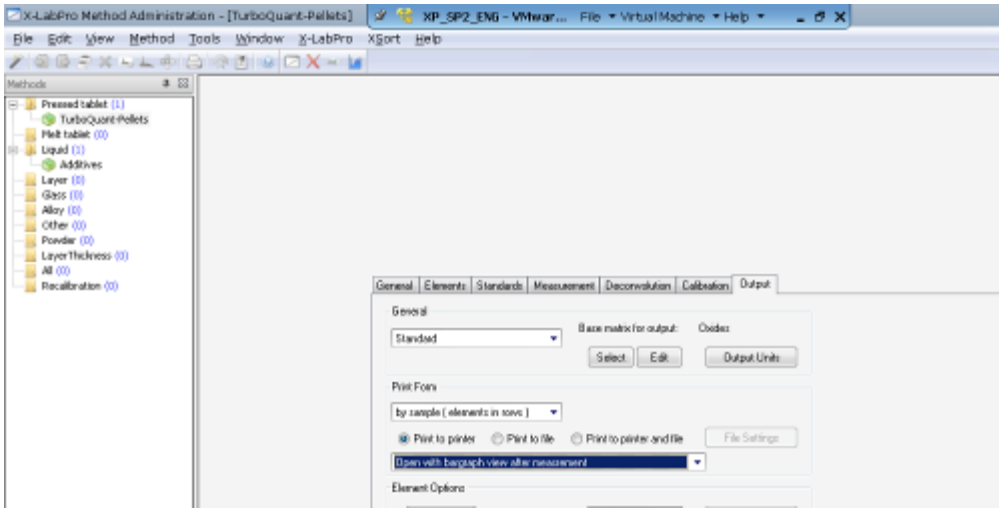
Certain applications require the compliance with a predefined set of concentration limits for one or more elements. The result viewer not only controls the compliance of the analytical result, it also presents it in a visual form with all relevant information included.

3.1 Selection of elements / definition of concentration limits

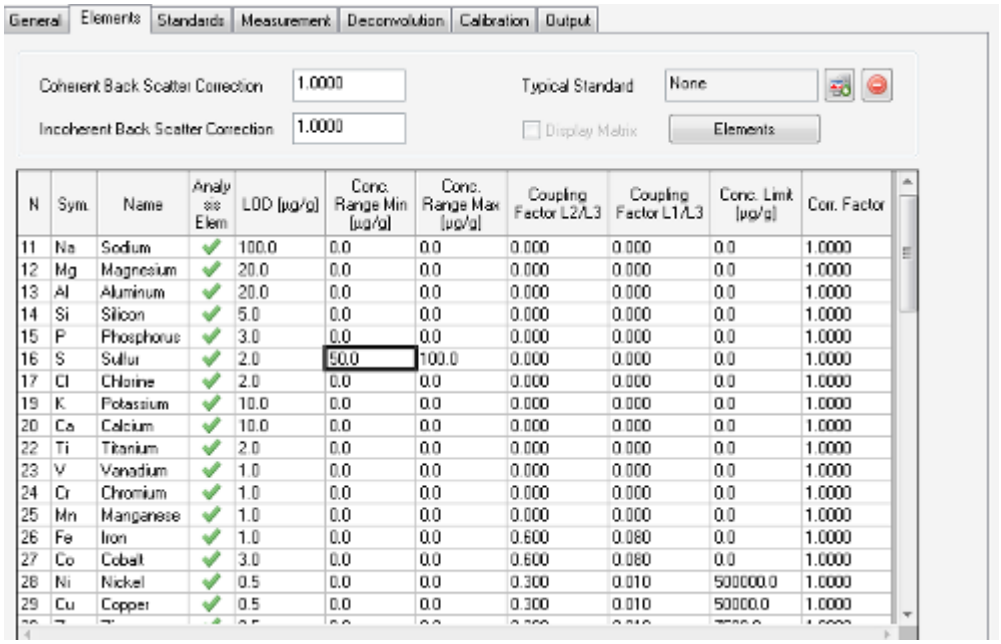
Open the “Method Administration” and select a method. In the tab “Output” – “Element Options” select the elements which have to be monitored.



To activate the Result viewer click on “Open Result View after Measurement”.

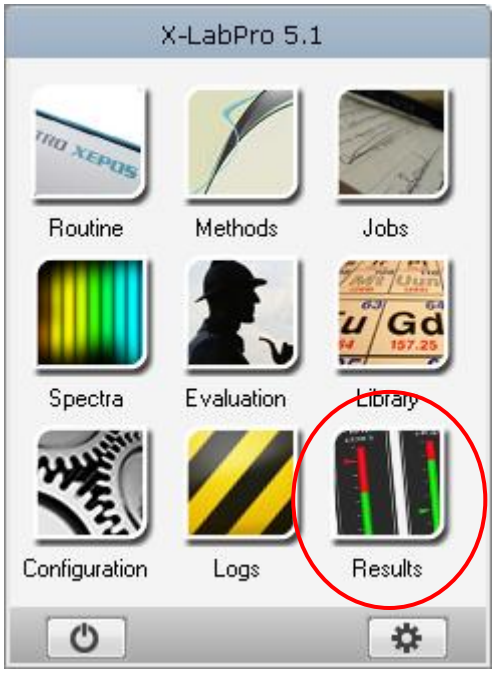


Select tab “Elements” and enter the minimum and maximum concentration range.



N	Sym.	Name	Analy ss Elem	LOD [µg/g]	Conc. Range Min [µg/g]	Conc. Range Max [µg/g]	Coupling Factor L2/L3	Coupling Factor L1/L3	Conc. Limit [µg/g]	Corr. Factor
11	Na	Sodium	✓	100.0	0.0	0.0	0.000	0.000	0.0	1.0000
12	Mg	Magnesium	✓	20.0	0.0	0.0	0.000	0.000	0.0	1.0000
13	Al	Aluminum	✓	20.0	0.0	0.0	0.000	0.000	0.0	1.0000
14	Si	Silicon	✓	5.0	0.0	0.0	0.000	0.000	0.0	1.0000
15	P	Phosphorus	✓	3.0	0.0	0.0	0.000	0.000	0.0	1.0000
16	S	Sulfur	✓	2.0	50.0	100.0	0.000	0.000	0.0	1.0000
17	Cl	Chlorine	✓	2.0	0.0	0.0	0.000	0.000	0.0	1.0000
19	K	Potassium	✓	10.0	0.0	0.0	0.000	0.000	0.0	1.0000
20	Ca	Calcium	✓	10.0	0.0	0.0	0.000	0.000	0.0	1.0000
22	Ti	Titanium	✓	2.0	0.0	0.0	0.000	0.000	0.0	1.0000
23	V	Vanadium	✓	1.0	0.0	0.0	0.000	0.000	0.0	1.0000
24	Cr	Chromium	✓	1.0	0.0	0.0	0.000	0.000	0.0	1.0000
25	Mn	Manganese	✓	1.0	0.0	0.0	0.000	0.000	0.0	1.0000
26	Fe	Iron	✓	1.0	0.0	0.0	0.600	0.080	0.0	1.0000
27	Co	Cobalt	✓	3.0	0.0	0.0	0.600	0.080	0.0	1.0000
28	Ni	Nickel	✓	0.5	0.0	0.0	0.300	0.010	500000.0	1.0000
29	Cu	Copper	✓	0.5	0.0	0.0	0.300	0.010	50000.0	1.0000

Open the “Results viewer”.



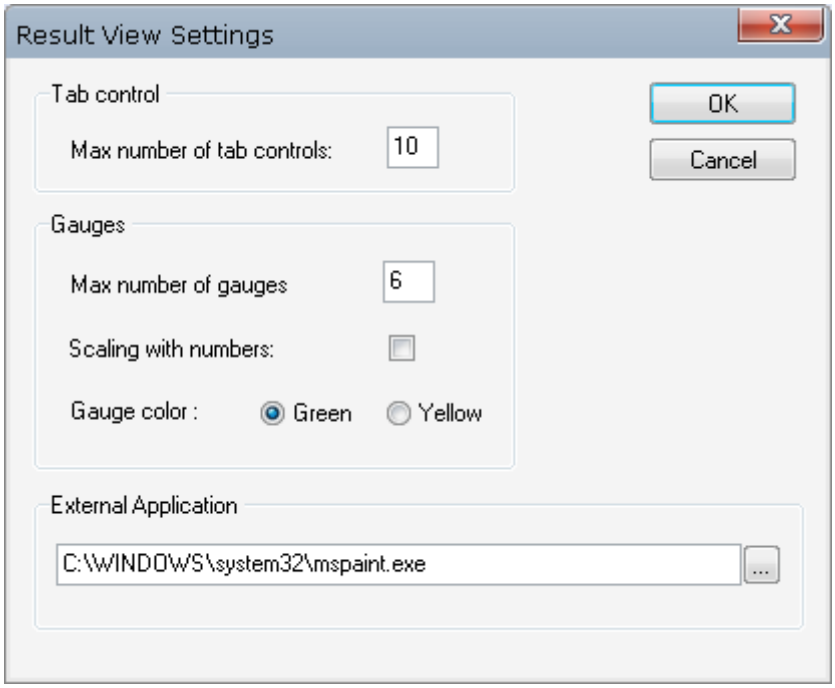
After a measurement is finished the results are displayed.

Green bar : defined concentration range

Green arrow : result within concentration range

Red arrow : result out of concentration range

If you would like to have further information, click on “Tools – Settings”.



Here you can choose if you would like a scaling on the bars and a different color for the concentration limits.

In the menu bar “View” you can either create a bitmap or open the bitmap in an external application.

4 Spectra Viewer

4.1 The Spectra Viewer

The Spectra Viewer is used to view and compare spectra measured by your X-LabPro software. To select spectra for the representation, the Spectra Viewer offers two possibilities:

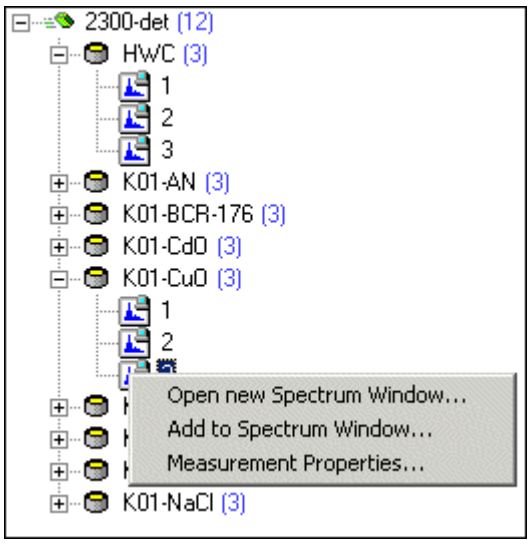
- The Tree Control
- The Selection Table

If at least one spectra window is shown, the following menus are enabled:

- File Menu
- View Menu
- Spectrum Menu
- MCA Menu
- Window Menu
- Help Menu

4.2 The Tree Control

In the left area of the Spectra Viewer it is possible to display the tree control. The tree control displays the methods or jobs; you can select it below the control use the tab control. The small blue number behind the methods (or jobs) shows the number of samples a method or job is containing. The small number behind the sample shows the number of measurements. The different sample types are displayed by different icons, just as the different measurement states (-, M, A).



4.2.1 How to Select Spectra for Representation

The usage of the tree control can be compared to the Windows Explorer. Use the following possibilities to select a spectrum for being displayed in a spectra window:

- A double click on a measurement opens the spectrum in a new spectra window.
- "Open new Spectrum Window" from the context menu (the context menu can be opened by clicking with the right mouse button on a measurement) opens the spectrum in a new spectra window.
- "Add to Spectrum Window" displays the selected measurement in an opened (and activated) spectra window.
- By clicking "Measurement Properties" important information about the measurement will be shown.

4.2.2 How to Enable/Disable the Tree Control

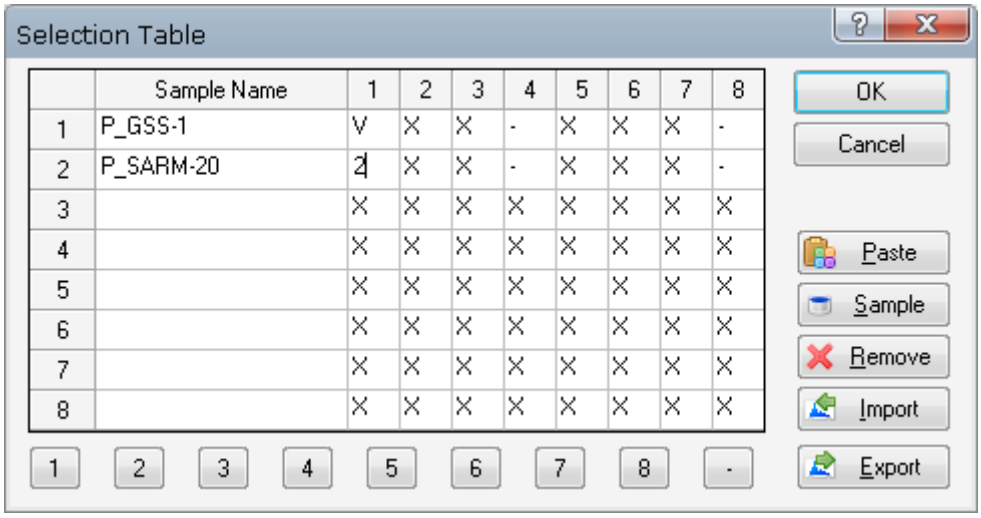
The tree control needs a lot of processor performance. Moreover, when opening the Spectra Viewer with an activated tree control, all databases must be scanned first. This needs a lot of time on older systems and it is possible that during a measurement, the databases will be locked. This causes possible errors and problems.

***Note*: If you are using an older PC system or if you want to use the spectra viewer during measurements, please disable the tree control.**

The tree control can be enabled or disabled by using the *Tree Control* menu point in the *View Menu*.

4.3 The Selection Table

Use the selection table to decide which spectra in which order will be shown in the selected spectra window. You can open the selection table by using the menu point *Selection Table* in the *Spectrum* menu. Moreover, you can use the shortcut "Ctrl+T" or the symbol in the toolbar.



4.3.1 Selecting Spectra

Use the command buttons to select spectra. Activate the referring cell in the *Sample Name* column before.

Paste Command Button
If you have copied sample(s) into the clipboard e.g. from the method window, use this command button to paste it into the selection table.

Sample Command Button
Click this command button to open a dialog for selecting a sample from a method or from a job.

Remove Command Button
Click this command button to delete a selected sample from the selection table.

Import Command Button
You can import samples from files by clicking on this command button..

Export Command Button
If a measurement is selected in the columns 1-6, you can export the sample data into a file.

1,2,3,4,5,6,7,8,- Command Buttons
Use this command buttons to define the order of the spectra.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

4.4 Menu Commands

4.4.1 Spectra Viewer Menu Overview

Menu overview

- File Menu
- View Menu
- Spectrum Menu
- MCA Menu
- Tools Menu
- Window Menu
- Help Menu
- System Menu

4.4.2 Commands in the File Menu

- **New**
  Creates a new spectra window.
- **Open**
  Use the *open* command to load an existing spectra window. This command will open a standard *Windows File Dialog* to select the spectra window.
  Shortcuts:

  Toolbar:
  Keyboard: CTRL+O
- **Close**
  Use the *close* command to close the selected spectra window. You will be promted to save the spectra data if the data contains any new information.
- **Save**
  Use this command to save the active spectra window to its current name and directory. If you want to change the name and directory of an existing spectra window before you save it, use the Save As command.
  Shortcuts:

  Toolbar:
  Keyboard: CTRL+S
- **Save as**
  Use this command to save and name the active spectra. The Spectra Viewer displays the Save As dialog box so you can name your spectra.

To save a spectra with its existing name and directory, use the Save command.

- **Print**
  Use this command to print the aktice spectra window.

- **Exit**
  Use this command to end the Spectra Viewer session. You can also use the *Close* command on the Application Control Menu. The Spectra Viewer prompts you to save documents with unsaved changes.
  Shortcuts:

  Mouse: Double click the application's Control menu Icon.

  Keys: ALT+F4

4.4.3 Commands in the View Menu

- **Toolbar**
  Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in the Spectra Viewer, such as File Open. A check mark appears next to the menu item when the toolbar is displayed.
  See Toolbar for help on using the toolbar.
- **Statusbar**
  Use this command to display and hide the Status Bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the Status Bar is displayed.
  See Status Bar for help on using the status bar.
- **ToolBox**
  Use this command to display or hide the tool window.
- **Tree Control**
  Use this command to display and hide the tree control. The tree control displays the methods or jobs.
- **Update Tree**
  Use this command to update the tree control after valid database changes have been made from X-LabPro. Use F5 as shortcut for this command.
- **Rebuild Tree**
  Use this command to rebuild the tree control completely from your X-LabPro database.

4.4.4 Commands in the Spectra Menu

The Spectra menu contents the following commands:

- **Selection Table**
  Select this menupoint to display the Selection Table Dialog Box.
- **Rotate**
  Select this menupoint to rotate the order of the spectra in the selected spectra window.

4.4.5 Commands in the Edit Menu

This menu is used to manipulate the displayed foreground spectrum and second spectrum. The abbreviation "MCA" stands for Multi Channel Analyzer. The menupoints in the menu are similar to the functions of an MCA. The menu is shown only in the Spectra window. The following menupoints are available:

- **Normalize to 2nd Spectrum**
  Select this menupoint to adjust the foreground spectrum to the second spectrum within a defined region (ROI). An adjustment factor is determined in the selected region using the least squares method. The channel contents in the foreground spectrum are then multiplied by this factor.
  The spectrum window will automatically switch to the ROI marking mode. Click the left mouse button in the spectral representation to select a ROI. The adjustment is automatically performed and the display is updated.
- **Normalite All to Foreground**
  Select this menupoint to adjust the background spectra to the foreground spectrum within a defined region (ROI). An adjustment factor is determined in the selected region using the least squares method. The channel contents in the are then multiplied by this factor.
- **Copy to Foreground**
  Select this menupoint to copy a selected region of the second spectrum into the foreground spectrum.
  The spectrum window will automatically switch to the ROI marking mode. Click the left mouse button in the spectral representation to select a ROI. The selected region of the second spectrum is automatically copied into the foreground spectrum and the display is updated.
- **Multiplicate 1st Spectrum...**
  Select this menupoint to multiplicate the foreground spectrum with a factor. A dialog will be opened to edit the factor.
- **Add 2nd Spectrum**
  Select this menupoint to add a selected region of the second spectrum from the foreground spectrum.
  The spectrum window will automatically switch to the ROI marking mode. Click the left mouse button in the spectral representation to select a ROI. The selected region of the second spectrum is automatically subtracted from the foreground spectrum and the display is updated.
- **Subtract 2nd Spectrum**
  Select this menupoint to subtract a selected region of the second spectrum from the foreground spectrum.
  The spectrum window will automatically switch to the ROI marking mode.

Click the left mouse button in the spectral representation to select a ROI. The selected region of the second spectrum is automatically subtracted from the foreground spectrum and the display is updated.

- **Edit Channel Contents**
  Select this menupoint to open the Edit Channel Contents dialog box. The impulse number can be manually edited for each channel in this dialog box. The display of the foreground spectrum is automatically updated.
- **Smooth Spectrum**
  Select this menupoint to smooth the foreground spectrum using a three point formula. The smoothened spectrum is automatically displayed as the foreground spectrum.
- **First Derivative**
  Select this menupoint to automatically calculate the first derivative of the foreground spectrum. The derivative is automatically displayed as the new foreground spectrum. Negative values or values smaller than 1 are displayed only in the linear representation display format.
- **Second Derivative**
  Select this menupoint to automatically calculate the second derivative of the foreground spectrum. The derivative is automatically displayed as the new foreground spectrum. Negative values or values smaller than 1 are displayed only in the linear representation display format.
- **Calculate Background**
  Select this menupoint to calculate a background for the foreground spectrum in the second spectrum. The Calculate Background dialog box opens. After the calculation, the calculated background is automatically displayed as the second spectrum.
- **Reset Foreground Spectrum**
  Select this menupoint to abandon any changes to the foreground spectrum. The original data for the measurement is newly read from the measurement databank when the spectrum is reset.
- **Reset 2nd Spectrum**
  Select this menupoint to abandon any changes to the second spectrum. The original data for the measurement is newly read from the measurement databank when the spectrum is reset.
- **Reset All Spectra**
  Select this menupoint to abandon any changes to all spectra. The original data for the measurements is newly read from the measurement databank when the spectrum is reset.
- **Assign Background**
  Select this menupoint to save the current spectrum as a background spectrum.

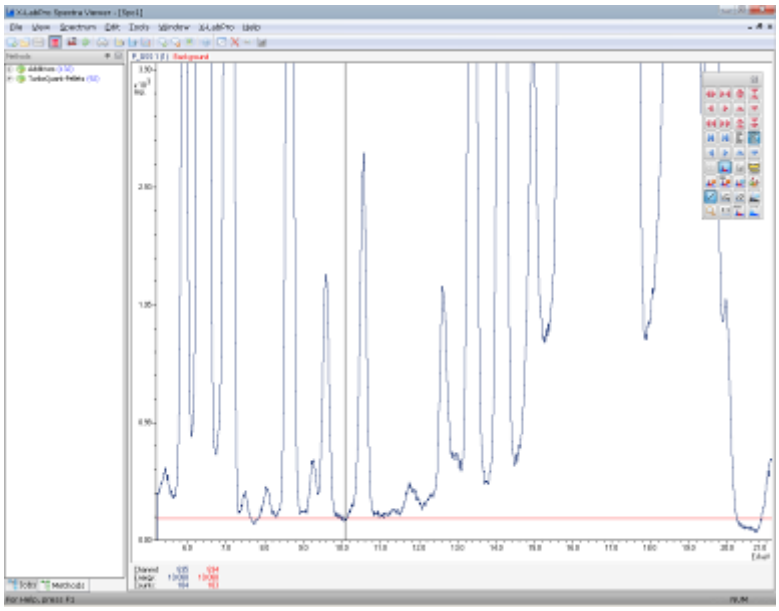
Note: The manipulations are always performed on the foreground spectrum, with one exception (Calculate Background).

4.4.6 Calculate Background Dialog Box

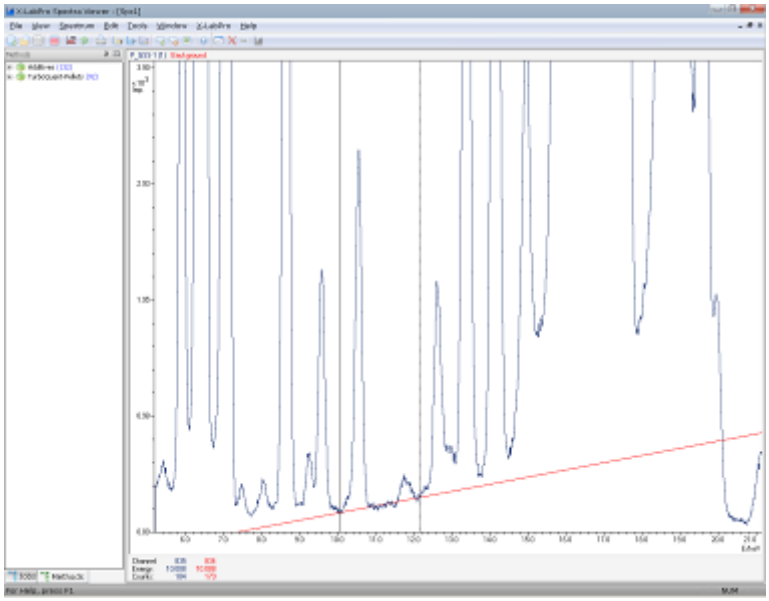
This dialog box is used to select the type of calculation to be used to calculate the background. This dialog box is opened with the Calculate Background menupoint in the MCA menu. The dialog box contains the following elements:

Background Type Group Box

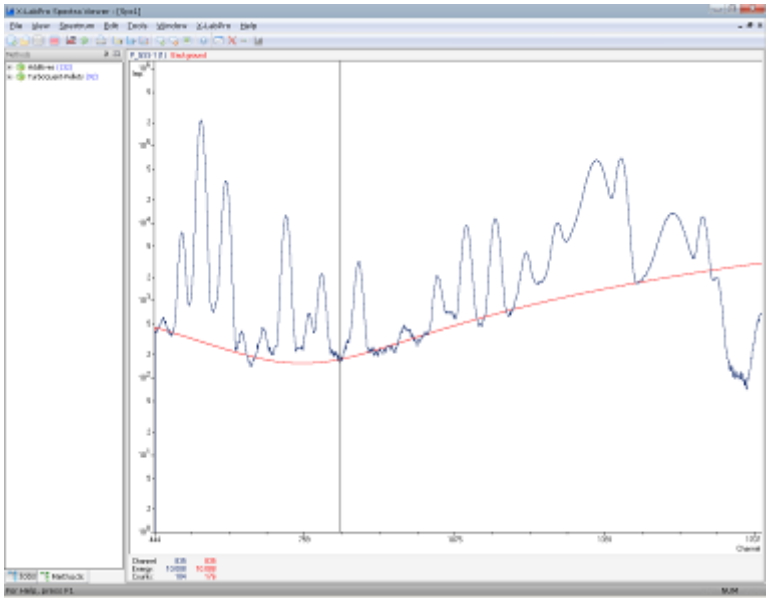
Constant Background Option Button
Select this option button to calculate a constant background. The background is calculated using the defined ROI. At least one ROI must be defined for a constant background. The following figure shows an example of a constant background:



Linear Background Option Button
Select this option button to calculate a linear background. The background is calculated using the defined ROI. At least two ROI must be defined for a linear background. The following figure shows an example of a linear background:



Quadratic Background Option Button
Select this option button to calculate a quadratic background. The background is calculated using the defined ROI. At least three ROI must be defined for a quadratic background. The following figure shows an example of a quadratic background:



OK Command Button
Click on this command button to close the dialog box. The background is calculated and carried into thesecond spectrum.

Cancel Command Button
Click on this command button to close the dialog box and cancel the procedure for calculating the background.

Note:

The calculated background is carried into the second spectrum. The calculated background can then be subtracted from a selected region of the foreground spectrum using the Subtract 2nd Spectrum menupoint in the MCA menu.

4.4.7 Edit Channel Contents Dialog Box

This dialog box is used to edit the impulse number for the channel at the position of the energy cursor for the foreground spectrum in the selected spectrum window. This dialog box is opened with the Edit Channel Contents menupoint in the MCA menu. The dialog box contains the following elements:

Channel Display Field
The number of the channel selected in the spectrum window is displayed in this display field.

Energy Display Field
The energy of the channel selected in the foreground spectra is displayed in this display field.

Impulse (old) Display Field
The number of impulses for the selected channel in the foreground spectrum is displayed in this display field.

Impulse (new) Text Box
Enter the new value for the number of impulses for the selected channel in this text box.

← (Left Arrow) Command Button
Click on this command button to select the previous channel. Changes in the impulse number for the currently selected channel are automatically carried into the foreground spectrum.

→ (Right Arrow) Command Button
Click on this command button to select the next channel. Changes in the impulse number for the currently selected channel are automatically carried into the foreground spectrum.

OK Command Button
Click on this command button to close the dialog box and carry the new value into the foreground spectrum.

Cancel Command Button
Click on this command button to close the dialog box and cancel the procedure for editing the channel contents.

Note: Select the Reset Foreground Spectrum in the MCA menu to reset any changes in the foreground spectrum.

4.4.8 Window Menu

This menu is used to switch between and arrange windows. The menu is displayed in every open window. The following menupoints are available:

- **Cascade**
  Select this menupoint to arrange open windows so that the title bar of each

window is visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.

- **Tile**
  Select this menupoint to arrange all of the open windows side by side so that all of them are visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.
- **Arrange Icons**
  Select this menupoint to arrange the icons within the application window.

4.4.9 Commands in the Help Menu

- **Contents**
  Select this menupoint to display a table of contents for the help system for the X-LAB^{Pro} program. In the help system, select the Contents command button below the menuline to show the table of contents.
- **Context Sensitive**
  Select this menupoint to display a context sensitive help text. This menupoint corresponds to the command button with a question mark in the toolbar.
- **Software**
  Select this menupoint to display a table of contents for the software description. Use of the operation and control software for the X-LAB energy dispersive x-ray fluorescence spectrometer is described in this section.
- **About XLSpcView**
  Show the version and copyrights of the Spectra Viewer.

4.5 Other

4.5.1 Toolbar

The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many functions used in the Spectra Viewer.

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Click To

	Create a new spectra window
	Open an existing spectra window. The Spectra Viewer displays the *Open* dialog box, in which you can locate and open the desired file.
	Save the active spectra window with its current name. If you have not named the document, the Spectra Viewer displays the *Save As* dialog box.
	Display or hide the Toolbox Window

	Opens the Selection Table Dialog Box
	Rotate the order of the spectra in the selected spectra window
	Print the actually spectra.
	Calculate the associated escape lines for the selected elements.
	Calculate the associated Pile-Up lines for the selected elements.
	Search for elements in the actually spectra.
	Insert a text at an arbitrary position.
	Delete one or all inserted text(s) from the spectral representation.
	Create a bitmap/jpeg file from the current spectral representation.
	Opens the Online Help.

4.5.2 Status Bar

The status bar is displayed at the bottom of the Spectra Viewer. To display or hide the status bar, use the Status Bar command in the View menu

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button.

Moreover the database reading status will be shown in the statusbar by a progress bar.

The right areas of the status bar indicate which of the following keys are latched down:.

Indicator Description

CAP	The Caps Lock key is latched down.
NUM	The Num Lock key is latched down.
SCRL	The Scroll Lock key is latched down.

4.5.3 Titlebar

The title bar is located along the top of a window. It contains the name of the application and the spectra window.

To move the window, drag the title bar. Note: You can also move dialog boxes by dragging their title bars.

A title bar may contain the following elements:

	Exit button.
	Maximize button.
	Minimize button.
	Name of the application.
	Name of the spectra window
	Applications icon.

4.6 Tool Window

4.6.1 Toolbox

The toolbox window offers a lot of functions to view and edit spectral representations. You can enable/disable this window by clicking the menu point *Toolbox* in the *View menu*. It may be freely moved around on the monitor. In this way, it is possible to move the window so that it does not interfere with your view of the portion of the spectrum that is being examined. The Toolbox window contains the following command buttons:

	Click on this button to stretch the displayed spectrum. At least 64 channels are always displayed.
	Click on this button to compress the displayed spectrum.
	Click on this button to stretch the display of the spectrum along the y-axis. The extent of the change depends on the type of display.
	Click on this button to compress the spectrum along the y-axis. The extent of the change depends on the type of display.
	Click on this button to shift the displayed spectrum in small steps to the left.
	Click on this button to shift the displayed spectrum in small steps to the right.
	Click on this button to shift the displayed spectrum in small steps upwards.

Click on this button to shift the displayed spectrum in small steps downwards.

Click on this button to shift the displayed spectrum in large steps to the left.

Click on this button to shift the displayed spectrum in large steps to the right.

Click on this button to shift the displayed spectrum in large steps upwards.

Click on this button to shift the displayed spectrum in large steps downwards.

Click on this button to move the Energy cursor one channel to the left. If the Energy cursor is not active, it is automatically activated by clicking on this command button.

Click on this button to move the Energy cursor one channel to the right. If the Energy cursor is not active, it is automatically activated by clicking on this command button.

Click on this button to switch to the channel representation.

Click on this button to switch to the energy representation.

Click on this cursor to move the Z-cursor to the element with the next, higher atomic number. If the Z-cursor is not active, it is automatically activated by clicking on this command button.

Click on this cursor to move the Z-cursor to the element with the next, lower atomic number. If the Z-cursor is not active, it is automatically activated by clicking on this command button.

Click on this cursor to move the Z-cursor to the next, higher shell; the element with the nearest energy is chosen. If the Z-cursor is not active, it is automatically activated by clicking on this command button.

Click on this cursor to move the Z-cursor to the next, lower shell; the element with the nearest energy is chosen. If the Z-cursor is not active, it is automatically activated by clicking on this command button.

Click on this button to display or hide the background grid.

Click on this button to turn display of the selected ROI on or off. Display of the ROI is automatically enabled after a ROI is defined.

Click on this button to turn display of the selected line markers on or off. Display is automatically activated when line markers are selected.

Click on this button to open the Select Elements dialog box in order to select the line markers to be displayed

Click on this button to open the Select Lines dialog box in order to select the line markers to be displayed.

Click on this button to delete the ROI at the current Energy cursor position.

Click on this button to delete all of the ROI in the displayed spectrum.

Click on this button to view data for the ROI data of the displayed spectra.

Click on this button to search for the lines at the current Energy cursor position.

Click on this button to activate the logarithmic representation of the spectrum.

Click on this button to activate the square root representation of the spectrum.

Click on this button to activate the linear representation of the spectrum.

Click on this button to reset the display of the spectrum to its original values.

Click on this button to switch to the magnify mode. You can choose an area to zoom in by using your mouse.

Click on this button if you want to switch the spectral representation to display one channel on one pixel.

Click on this button to enable the ROI marking mode. Display of the ROI is automatically enabled after a ROI is defined.

The cursor keys may also be used to move the Energy cursor.

4.6.2 Select Lines Dialog Box

You can use this dialog box to manage all displayed lines of your spectra window. You can choose lines from a list of all available lines or from a list of filtered lines:

Available Lines List Box
Shows all available Lines or lines filtered by element and/or by energy. Use the checkboxes "Filter By Element" and "Filter By Energy" to use the filter options.

Filter By Element Check Box
Enables a filter for displaying only lines belonging to the selected elemnt. You can enter an element atomic number or select an element from the periodic table.

Filter By Energy Check Box
Enables a filter for displaying only lines in a defined area of energy. Enter your energy limits in the text fields.

Selected Lines List Box
Shows the lines selected for being displayed in the spectra window.

Insert Command Button
Copies a selected line from the "Available Lines" list box to the "Selected Lines" list box.

Remove Command Button
Deletes the selected line in the "Selected Lines" list box.

Remove all Command Button
Deletes all lines in the "Selected Lines" list box.

Show Line Marker Text Check Box
Enables/disables the display of the line name for the selected line.

Show Element Symbol Only Check Box
Switch the announcement of the line designation in the spectrum representation on or off.

Show Escape Lines Check Box
Switch the announcement of the Escape Lines in the spectrum representation on or off.

Show Pile-Up Lines Only Check Box
Switch the announcement of the Pile-Lines in the spectrum representation on or off.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

5 Method Administration

The Method Administration is used to do all settings for the methods in the X-LabPro software. Create, edit or delete methods or the assigned standard samples here. You get information about the methods in general and about their standard samples or measurements. Settings for deconvolution or calibration may also be done.. The Method Administration offers two possiblities to navigate through and use the application:

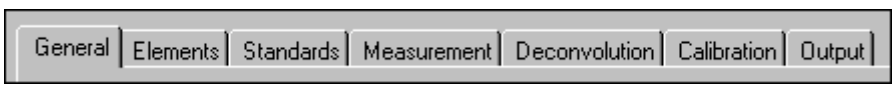
- The Tree Control
- The Method Window

If at least one method is opened, the following menus are enabled:

- File Menu
- Edit Menu
- View Menu
- Method Menu
- Tools Menu
- Window Menu
- X-LabPro Menu
- Help Menu

5.1 The Method Window

In the right area of the Method Administration the Method Window is displayed. Here you get some different property pages which guide you to get information and do settings dependant on the opened method. Click on the title of a property page to open it.



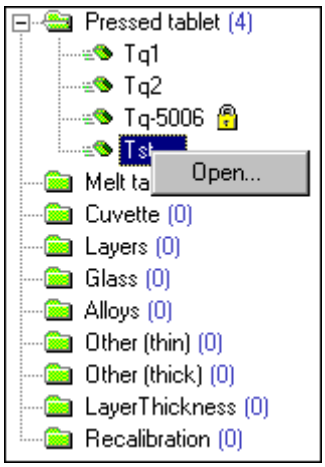
- *General*: This page includes general information about the opened method like global settings, dilution, normalization and additional settings. Moreover, you can finalize the method here.
- *Elements*: You may choose the elements you want to analyse and do the settings on this page.
- *Standards*: Get a table of the assigned standard samples of the opened method and information about these standard samples.You may also create, edit or delete standards here.
- *Measurement*: On this page you get information or do settings for the number and type of measurements.
- *Deconvolution*: This page offers you the possibility to do settings for the deconvolution. *Calibration*: Do the settings for the calibration on this page.
- *Output*: Do the settings for the printer output on this page.

If you select another page of the Method Window by clicking the title of this page and if you have changed values or parameters, you will be prompted to confirm the changes. In this case the changes will be written to the database immediately.

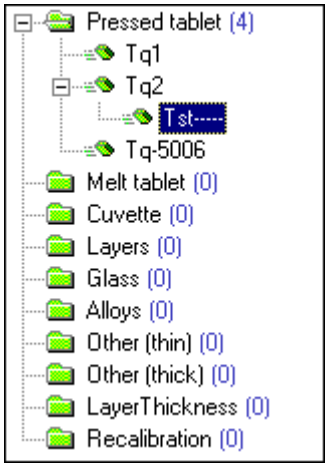
See also:
Method Administration
Method Administration (Tree Control)

5.2 The Tree Control

In the left area of the Method Administration the tree control is displayed. Here you find all methods ordered by their sample types. Click on the small cross next to an icon to open a sample type folder and get a list of the methods. The small blue number behind the description of a folder shows the number of methods the folder is containing. A padlock behind the name of a method indicates that the method is finalized. Double click on a method to open it in the Method Window. You may also use the context menu to open a method: Right click on a method and select OPEN.



You may sort the different methods in a hierachy by using the option *Subclass Methods* of the File Menu. While selected, this option offers you to drag a method with a left mouse click and drop it as a child in the tree.



See also:
Method Administration
Method Window

5.3 General Page

The General Page of the Method Window is used to set the parameters for the method, dilution material and normalization in different group boxes. You may also finalize the method currently selected or do an automatic recalibration.

Global Settings Group Box
The global method settings are displayed and can be changed with the dialog elements in this group box. The individual elements have the following meanings:

Method Name Text Box
The name of the currently selected method is displayed and can be changed in this text box.

Created by Text Box
The name of the user who created the method is displayed and can be changed in this text box.

Sample Type Drop-down List Box
The sample type for which the method was defined is displayed and can be changed in this drop-down list box.

Sample State Drop-down List Box
The sample state to which the method is assigned is displayed and can be changed in this drop-down list box. The parameters depand on the pre-defined sample state. To define/edit sample types/states use the configuration editor.

Description Text Box
A short description of the method is displayed and can be changed in this text box.

Matrix for Calib. Text Field
The chosen matrix for calibration is displayed in this text field.

Select Button
Click on this button to select a matrix for calibration. The matrices can be defined in the configuration editor.

Edit Button
Click on this button to create or edit a matrix for calibration

Mathematics Drop-down List Box
The mathematical method for the calculation is displayed and can be changed in this drop-down list box.

Option Drop-down List Box
Use this drop-down to select what kind of method you want to create (e.g. recalibration).

Use external concentration as Drop-down List Box
The meaning of the external concentration is displayed and can be changed in this drop-down list box.

Dilution Group Box
The information about the used dilution is displayed and can be changed with the dialog elements in this group box. The individual elements depend on the selected sample state and can be pre-defined in the configuration editor.

Dilution Material Drop-down List Box
The dilution material of the currently selected method is displayed and can be changed in this drop-down list box.

Sample Mass Text Box
The sample mass (in g) of the currently selected method is displayed and can be changed in this text box.

Dilution Mass Text Box
The dilution mass (in g) of the currently selected method is assigned is displayed and can be changed in this text box.

Sum/Factor Display Fields
The sum of the sample mass and the dilution mass and the part of the sample mass of the sum of both is displayed in this display field.

Additional Settings Group Box
The additional method settings are displayed and can be changed with the dialog elements in this group box. The individual elements have the following meanings:

Sample Diameter Text Box
The sample diameter (in mm) is displayed and can be changed in this text box. The default diameter depends on the selected sample state and can be pre-defined in the configuration editor.

Cuvette Foil Drop-down List Box
The type of the cuvette foil of the method is displayed in this drop-down list box.

Protection Foil Drop-down List Box
The type of the protection foil of the method is displayed in this drop-down list box.

Note: The foils can be defined in the configuration editor.

Dust Protection Foil / Liquid Protection Cup Radio Button
Select with this radio button the usage of the protection foil. If you select Dust Protection Foil the Routine Dialog will ask for inserting the foil.

Standard for Comparison Display Field
The standard for comparison of the method is displayed in this display field. To select or change the standard click on the button at right. You will be prompted to choose a standard. Click on the cross to delete the selection.

Normalization Group Box
The settings of the normalization are displayed and can be changed with the dialog elements in this group box. Choose the type of the normalization between the following dialog elements:

No Normalization
Select this option if you don´t want to normalize. *See*: Normalization.

Use MSK Calibration
Select this option to normalize via MSK Calibration.

Normalize Results
Select this option to normalize the results. You are asked to enter the normalization concentration by one value or a bandwith.

Difference Element
Select this check box to enter an element which influences the sample but which isn´t measurable. This can be used to tell the mathematical procedure, what's the "non-visible" part of the sample. You may enter the number of the element in the text box below or left click on the button PTE to get the periodic table of elements where you can choose one element.

Finalize Button
To finalize your method click this button. *Note*: A finalized method cannot be modified further.

See also:
Method Administration
Method Window

5.4 Element Page

You may choose the elements you want to analyse and do the settings on this page of the Method Window. This page offers the following dialog elements:

Coherent Back Scatter Correction Text Box
The intensity correction factor for the coherent back scatter correction is displayed and can be changed in this text box.

Incoherent Back Scatter Correction Text Box
The intensity correction factor for the incoherent back scatter correction is displayed and can be changed in this text box.

Typical Standard Display Field
The typical standard sample for this method is displayed in this display field. To

select or change the standard sample click on the button at right. You will be prompted to choose a standard sample. Click on the cross to delete the selection.

Elements Button
Click on this button to select the elements you want to analyse. The Select Elements dialog box will be opened and shows a periodic table of elements. Here you may select the desired elements. All of the elements that are to be expected for the samples to be measured should be selected.

Display Matrix Check Box
Activate this check box to enable the matrix presentation of the selected elements and the displayed values.

Elements Table
In the table below the selected elements are listed. Do the settings for the different elements here. The table contains the following columns:

N Column
The atomic number of the element is displayed in this column.

Sym. Column
The element symbol (or its chemical bond) of the element is displayed in this column.

Name Column
The name of the element is displayed in this column.

Analysis Elem Column
Select this option to include the element to the analysis. A check mark appears if the option is selected.

LOD [µg/g] Column
This column shows the value for the Limit of Detection of the element. You may enter a new value. Valid entries lie in the range between 0 and 10000 µg/g.

Conc. Range Min [µg/g] and Conc. Range Max [µg/g] Columns
It is possible to calculate up to three calibrations for different concentration ranges. Control of selection of the range is conducted using the min and max concentration limit for the respective calibration. Enter the desired range in this two columns. If only one calibration is to be calculated, then select the concentration limits for this range so that all possible cases fall within one range.

Conc. Limit [µg/g] Column
Enter the concentration limit for consideration of the lower shell for the selected element in this column.

See also:
Method Administration
Method Window

5.5 Standard Page

On this page of the Method Window all standard samples assigned to the opened method are listed in a table. You may edit the standard samples by using the menu points in the Edit Menu, the buttons of the toolbar or the menu points of the context menu. The context menu will be opened by right clicking on a standard sample, it contains the same menu points as the Edit Menu.. Please see Edit Menu for additional information.

Standards Table
In the table below the standard samples are listed. The table contains the following columns:

Name Column
The name of the standard sample is displayed in this column.

Description Column
The description of the standard sample is displayed in this column.

Status Column
The measurement status of the standard sample is displayed in this column.

Creation Date Column
The creation date of the standard sample is displayed in this column.

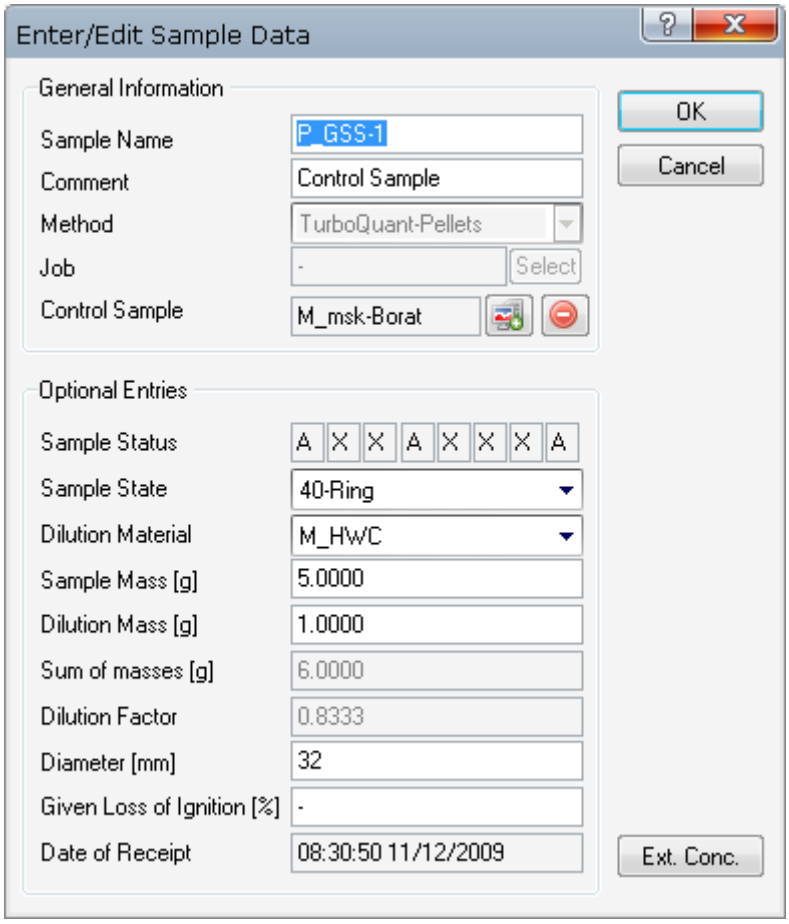
Evaluation Date Column
The evaluation date of the standard sample is displayed in this column.

Dilution Column
If the standard sample is using a dilution, a check mark appears in this column.

Backg. Column
If the standard sample is a background sample, a check mark appears in this column.

See also:
Method Administration
Method Window
Method Administraiton (Edit Menu)

5.5.1 The Enter/Edit Sample Data Dialog



This dialog box is used to enter and edit data for a sample or a standard sample. The dialog box contains the following elements:

General Information Group Box

Sample Name Text Box
Enter the sample name (up to 250 characters) in this text box.

Comment Text Box
Enter an additional description (up to 20 characters) for the sample here. This text box does not have to be filled in.

Method Drop-Down List Box
The name of the method to which the sample is assigned is displayed in this display field. When editing a sample (not standard) you can select a method here.

Job Drop-Down List Box
The sample can be assigned to a job in this list box. This command is not active for the definition of a standard sample, because standard samples are always assigned to a single method. If the dialog box is opened from the Job Manager, then the name of the currently selected job is automatically entered.

Control Sample Display Field and Buttons
The name of the sample for comparison (control sample) is displayed in this display field. Use the button to select a control sample spectrum. Use the button to remove your selection and reset the display field to "None". The spectrum of the control sample is shown as the second spectrum in the Routine Dialog (Measured Spectrum) during the measurement.

Optional Entries Group Box

Measurement Status 1 bis 6 Display Fields
The measurement status of the sample is shown in these fields.

Sample State Drop-Down List Box
Select the desired sample state in this drop-down list box. The possible sample states can be changed in the Sample Settings dialog box.

Dilution Material Drop-Down List Box
Select the name of the desired dilution material in this drop-down list box. The possible dilution materials must be defined in the selected method as standard samples that are marked as dilution materials. If no dilution materials have been defined, the text "none" is displayed.

Sample Mass Text Box/Display Field
Enter the sample mass (in g) in this text box. Whether this field or the three following fields are active or not, depends on the settings in the Sample Settings dialog box. It is possible to choose between two variations: The entry of sample and dilution mass or the entry of total mass and dilution factor. For each option, the other quantities are automatically calculated.

Dilution Mass Text Box/Display Field
Enter the dilution mass (in g) in this text box (see "Sample Mass Text Box/Display Field" for additional information).

Sum of Masses Text Box/Display Field
Enter the sum of the masses for the sample (in g) in this text box (see "Sample Mass Text Box/Display Field" for additional information).

Dilution Factor Text Box/Display Field
Enter the dilution factor in this text box (see "Sample Mass Text Box/Display Field" for additional information).

Diameter Text Box
Enter the sample diameter (in mm) in this text box.

Given Loss Of Ignition Text Box
Enter the given value for the loss of ignition (in percent) in this text box. If you do not want to set a value for the loss of ignition, enter "-1" or simply a dash. The loss of ignition is interpreted to be 0% if a zero is entered.

Date of Receipt Text Box
Enter the date of receipt for the sample into your laboratory in this text box. The date is printed with the printout of the results. When a new sample is entered, this field is automatically filled with the current date.

Ext. Conc.
Click on this command button open the Edit External Concentrations for Sample Dialog Box.

OK Command Button
Click on this command button to close the dialog box and save the modified or newly entered sample.

Cancel Command Button
Click on this command button to close the dialog box. New samples or changes to an existing

See also:

Edit Menu (Job Manager)
Edit Menu (Method Development)

5.5.2 Given Concentrations Dialog Box

This dialog box is used to enter and edit the given (e.g. certified) concentration for a standard sample. This dialog box is opened with menu point Given Concentrations of the Edit Menu (Method Administration) or via the context menu of the Standards Page (Method Window). The dialog box contains the following elements:

General Information Group Box

Sample Name Display Field
The name of the selected standard sample is displayed in this display field.

Comment Display Field
The comment of the selected standard sample is displayed in this text box.

Sample State Display Field
The state of the selected standard sample is displayed in this display field. The possible sample states can be changed in the Sample Settings dialog box.

Dilution Material Display Field
The name of the assigned dilution material is displayed in this display field.

Sample Status Display Field
The measurement status is displayed in this field.

Sample Mass Display Field
The sample mass is displayed in g in this display field.

Dilution Mass Display Field
The dilution mass is displayed in g in this display field.

Dilution Factor Display Field
The dilution factor calculated from the sample and dilution masses is displayed in this display field.

Sample Specification Group Box

Average Atomic Number Calibration Check Box
Mark this check box if the selected standard sample is to be used for the Average Atomic Number Calibration.

Mass Attenuation Coefficient Calibration Check Box
Mark this check box if the selected standard sample is be used for the Mass Attenuation Coefficients Calibration.

Layer thickness standard Check Box
Mark this check box if you want to use a layer thickness calibration. Note that the following elements will be enabled and overwrite other ones.

Substrat Display Field
The name of the assigned substrat is displayed in this display field. This display field overwrites the *Dilution Material Display Field* of the *General Information Group Box*.

Density Display Field
The density of the standard sample is displayed in this display field. This display field overwrites the *Sample Mass Display Field* of the *General Information Group Box.* Further the *Dilution Mass* and *Dilution Factor Display Fields* are disabled.

Substrat Check Box
Mark this check box if the selected standard sample is to be used as a substrat. This Check Box overwrites the *Dilution Material Check Box* of the *Sample Specification Group Box*.

Layer Thickness [nm] Text Box
Enter the layer thickness in this text box. This text box is added to the *Settings for given conc. Group Box*.

Standard Type Drop-Down List Box
Select in this Drop-Down List Box the sample type if the selected standard sample is to be used as one of the following sample types:

Dilution Material (D)

Validation Sample (V)

Method Recal Sample (M)

Intercept Recal Sample (I)

Settings for given conc. Group Box

Bonds Check Box
Mark this check box if you want to enter the concentrations as bond concentrations. The bonds are set in the Edit Chemical Bonds dialog box . When entered, the concentrations for the bonded elements are automatically, proportionally entered.

Output Ele. Only Check Box
Mark this check box if you want to display only the output elements. Note: The elements H, C, N and O are always shown.

Typical Unit Drop-Down List Box
Select the typical mass unit for entry of the given values for the standard sample.

Sum of Conc. Display Field
The sum of the entered given concentrations is displayed in % in this display field.

Concentration Values Group Box

In the Concentration Values Group Box you find a table with the following columns:

Z Column
The atomic number of the selected element is displayed in this column. Row 0 includes the LOI (loss of ignition).

Symbol Column
The element symbols of the selected element is displayed in this column.

Element Column
The element names of the selected element is displayed in this column.

Conc. Column
Enter the given concentrations of the selected element in this column.

Error Column
Enter the absolute errors of the given concentrations of the selected element in this column.

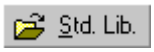
Level Column
Select certification level for the selected element for the standard sample in this drop-down list box.

Emp. 1, 2, 3, Fund. 1, 2 and Std. Columns
Select this options by a left mouse click if the standard sample should be used for the calibration (Compton/empirical calibration, fundamental parameter calibration and recalibration) for the various evaluation methods for the selected element. A check mark appears in the field if the option is enabled.

Std. Lib. Command Button (Save)

Click on this command button to store the data for the standard sample in the library of standards.

Std. Lib. Command Button (Load



Click on this command button to load the data of a standard sample in the library of standards.

Reset Command Button
Click on this command button to reset the settings for the selected standard sample to the default values stored in the library of standards . The name of the standard sample must be the same as the name of an entry in the library of standards . If this is not the case, all of the concentrations are set to zero. A message to this effect is displayed.

OK Command Button
Click on this command button to close the dialog and store the settings that have changed.

Cancel Command Button
Click on this command button to close the dialog without storing changes to the settings.

5.6 Measurement Page

On this page of the Method Window you can edit the settings for the measurements of the standard samples of the selected method. The page contains the following elements:

General Settings Group Box
Do the general settings for the measurements in this group box. The different elements have the following meanings:

Measurements 1-8 Check Boxes
Here you can select how many and which measurements should be assigned to a standard sample of the selected method. A check mark appears if the check box is selected.

Measurement Type Drop-down List Box
Select the measurement type of the standard samples in this Drop-down List Box.

Sample Rotation Check Box
If this check box is enabled the sample will be rotate during a measurement

Quick Start Check Box
If the Quick Start feature is enabled, gas flush or vacuum pumping will be done during the first measurement. When disabled, it will be done before the first measurement.

Measurements Pages
For each measurement selected in the General Settings Group Box you may do individual settings. Left click on the title of the measurement´s page you want to edit. The measurement pages offer you the following group boxes.

Detection System Group Box
Do the settings for the Detection System in this group box. The group box contains the following elements:

Channels Drop-down List Box
Select the number of channels for the measurement in this drop-down list box. Valid entries are 1024, 2048 and 4096.

Peak Time [µs] Drop-down List Box
Select the peak time that is to be used for the selected measurement in this drop-down list box.

Zero Peak Rate [cps] Drop-down List Box
Select the zero peak rate that is to be used for the selected measurement in this drop-down list box.

Energy Range[keV] Drop-down List Box
Select the energy range that is to be used for the selected measurement in this drop-down list box.

Target Drop-down List Box
Select the target to be used for the selected measurement in this drop-down list box.

Generator Control Group Box
Do the settings for the Generator Control in this group box. The group box contains the following elements:

Voltage Group Box
Use the slider to set the tube voltage for the selected measurement. The values that can be currently set, depending on the tube characteristic line, are displayed at the end of the scroll bar. Valid entries lie in the range between 8 kV and a value that can be set in the Instrument Control Settings dialog box.

The currently set tube voltage is displayed in kV in the text box. A new value for the voltage can also be entered in this field. If the value "zero" is entered for the voltage and for the current, the measurements are conducted with out high voltage. This can be useful for tests or for measurements with a nuclide source.

Current Group Box
Use the slider to set the tube current for the selected measurement. The values that can be currently set, depending on the tube characteristic line, are displayed at the end of the scroll bar. Valid entries lie in the range between 8 and 80 mA.

The currently set tube current is displayed in mA in the text box. If the value "zero" is entered for the voltage and for the current, the measurements are conducted with out high voltage. This can be useful for tests or for measurements with a nuclide source.

Mark the Current Regulation Check Box to set automatically the current of the measurement by evaluating the best value.

Measurement Time Limit Check and Group Box
Mark this field and group to end the selected measurement after a given maximum time has elapsed. Measurement limited by time can be combined with measurement by impulse number; the measurement is ended as soon os one of the conditions has been met. You are asked to do some further settings:

Measurement Time Text Box
Enter the default time for the maximum measurement time in this text box when the measurement is to be limited by time. Valid entries lie in the range between 0 and 200000 s.

Measurement Pulse Limit Check and Group Box
Mark this field and group to end the selected measurement after a given maximum impulse number has been reached in the given window (between first and last channel). You are asked to do some further settings:

No. of Impulses Text Box
Enter the maximum impulse number in this text box when the measurement is to be limited by impulse number. The measurement is ended when the sum of the impulses in the given window reach this number.

First Channel Text Box
When the measurement is to be limited by impulse number, enter the first channel

for the window in which the impulses are to be summed in this text box. Valid entries lie in the range between 1 and 1024 and must be smaller than or equal to the entry for the last channel.

Last Channel Text Box
When the measurement is to be limited by impulse number, enter the last channel for the window in which the impulses are to be summed in this text box. Valid entries lie in the range between 1 and 1024 and must be larger than or equal to the entry for the first channel.

See also:
Method Administration
Method Window

5.7 Deconvolution Page

Use this page of the Method Window to do the settings for the deconvolution. This page contains the following three property pages:

Number of background spectra Drop-Down List Box
Set the number of background spectra used in this drop-down list box. Since Version 3.0 the background spectra are stored in samples named Background_xx. The switchover between regions is set for each sample by the scattering ratio. The default for the number of background spectra is 3 (for light, medium and heavy sample matrices). A maximum of 6 different background spectra can be used. To use more than one background it is necessary that a Compton target is used for the first measurement and the selected mathematics is Ext. Compton, Spectro or Compton/Rayleigh.

Edit Limits Command Button
Click on this command button to open the Limits for Background Spectra Switchovers dialog box in order to change the scattering ratio for the switch between the various background spectra.

Property Pages
Further you get some property pages: The general page and one page for each measurement.

General Property Page
This page shows a table with all elements selected on the Elements Page. It gives an overview about the settings on the n Measurement tables. For example a 2,3 in the Intensity column of the row of element 11 means that for the measurements number 2 and 3 the option Intensity of the element number 11 is selected. You cannot edit the table on this page, it is created to give you an overview. The table contains the following columns:

N Column
The atomic number of the element is displayed in this column.

Sym. Column
The element symbol of the element is displayed in this column.

Name Column
The name of the element is displayed in this column.

Intensity Column
This column shows for which measurement and element the Intensity option is selected.Click on this command button to open the Select Elements dialog box. This dialog box is used to select the elements for which intensities are to be determined for the selected measurement. Individual elements can be selected for multiple measurements. Only elements that have been previously defined for the respective measurement as deconvolution elements can be selected.

Concentration Column
This column shows for which measurement and element the Concentration option is selected.

Measurement n Property Page
On this page you may do the individual settings for each measurement. The page contains the following elements:

Element Table
This table shows all intensity elements assigned to the measurement n. You may change the selection by clicking the Elements Button. The table contains the following rows:

N Column
The atomic number of the element is displayed in this column.

Sym. Column
The element symbol of the element is displayed in this column.

Name Column
The name of the element is displayed in this column.

Conc Column
Click on the check point in this column to select an element which concentrations are to be determined for the selected measurement. Each element can be selected for only one measurement. A number behind a check point indicates that the choosen element is already selected by the measuremment with the corresponding number.

Line Column
In this column you select the line to be used for the deconvolution in the drop-down list box. The type of line that should be selected depends on the type of excitation and the selected element. The following line types are available:

K-Alpha
K-Beta
L-Alpha
L-Beta
M-Alpha
M-Xi

Deconvolution Column
In this column you select the deconvolution strategy to be used for the deconvolution in the drop-down list box. The following deconvolution strategies are available:

Summation
The channel contents in the given deconvolution region are summed with this method. The K-alpha line should be used for elements with an atomic number > 21; the L-alpha line for elements with atomic numbers > 56. The lines are not subtracted from the spectrum. This strategy should only be used when no peak overlaps are expected.

Series Fit
This method is used when other methods cannot be used.

Line Fit
If the K-alpha or an L-alpha line (for elements with N > 56) is without overlaps, but the secondary lines are overlapped with K-alpha or L-alpha lines from other elements, then this overlap can be removed by determining the height of the lines that are not overlapped using a model adjustment. The heights of the secondary lines are calculated from the model spectrum and subtracted from the measured spectrum. The energetically next highest main line remains, without overlaps, in the spectrum. Main lines with more than 500 impulses are additionally used to standardize the energy-channel relationship with this method.

Example:
Evaluation of a Cr-Mn-Fe-Spektrum. The Mn K-alpha line is overlapped by the Cr K-beta line. The Fe K-alpha line is overlapped by the Mn K-beta line. Beginning with Cr, all of the elements can be processed with this method.

Line Fit with Standard
This method is similar to the line fit method, however, main lines with more than 3000 impulses are used for a width-energy relationship standardization in addition to an energy-channel relationship standardization.

Elements Button
Click on this command button to open the Select Elements dialog box. Select the elements to be considered with the selected measurement in this dialog box. These elements are selected as deconvolution elements for this individual measurement. All of the elements that are to be expected for the samples to be measured should be selected.

Deconvolution Region Button
Click on this command button to open the Select Deconvolution Regions dialog box. The deconvolution regions for the respective measurement can be set in this dialog box.

Background Region Button
Click on this command button to open the Select Background Regions dialog box. The background regions for the respective measurement can be set in this dialog box.

Normalization Region Button
Click on this command button to open the Select Normalization Regions dialog box. The normalization regions for the respective measurement can be set in this dialog box.

Iron Cobalt Corr. Check and Text Box
Mark this check box to activate the optional iron-cobalt correction. This is

necessary when there is a high iron concentration and iron and cobalt are to be deconvoluted in the same measurement. Enter the correction factor for the iron-cobalt correction in the enabled text box.

Target Name Display Field
The name of the target selected for the measurement is displayed in this display field.

Use Optimization Check Box
Mark this check box to enable the deconvolution optimization during the sample evaluation.

Voltage Display Field
The voltage selected for the measurement is displayed in this display field.

Deconvolution cycles Text Box
In this text box you determine how often the deconvolution will be repeated.

See also:
Method Administration
Method Window

5.7.1 Limits for Background Spectra Switchovers Dialog Box

This dialog box is used to set the limits for the switchovers for the various possible background spektra. The dialog box is opened with the Edit Limits command button on the Deconvolution Page of the Method Window of the Method Administration. The dialog box contains the following elements:

Scattering ratio for switchover to spectrum nText Boxes
Enter the the scattering ratio for which the nth background spectrum should be used in the respctive text boxes. The switchover occurs from large to small values. For 3 background spectra, the default entry is, for example, 4.1 for spectrum 2 and 1.5 for spectrum 3. In this way, samples with a scattering ration larger than 4.1 are evaluated with the first background spectrum; samples with a scattering ratio between 4.1 and 1.5 with the second background spectrum; and samples with smaller scattering ratios with the third background spectrum.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

5.8 Calibration Page

Use this page of the Method Window to do the settings of the calibration parameters. The page contains the three following property pages:

The method administration offers the following calibration models:

- Mass Attenuation Coefficient

- Extended Compton
- Fundamental Parameter Model
- Lucas Tooth/Price
- Spectro
- Compton/Rayleigh
- Layers

You will see different dialog elements depending on the selected calibration model:

Standards Property Page
The Standards Property Page shows a table which contains the folloing columns:

N Column
The number in this column shows how often a standard sample was used for the calibration. An empty field means that the standard sample was not used. You may enter numbers between 1 and 5 to weigh the different standard samples.

Standard Column
The name of an assigned standard sample is displayed in this column.

Intensity Column
The value of the intensity determined from the measurement is displayed in this column.

Given Column
The value of the given concentration/MAC is displayed in this column.

Calculated Column
The value of the calculated concentration/MAC is displayed in this column.

Difference Column
The value of the calculated difference (calculated - given) is displayed in this column.

Parameters Property Page

This page displays a table with the assigned parameters. It contains the following columns:

No. Column
The number of the parameter is displayed in this column.

Parameter Column
The name of the parameter is displayed in this column.

Value Column
The value of the parameter is displayed in this column.

Calibration Diagram Property Page

On this page you get two diagrams with the following meanings:

Upper Diagram
This diagram displays the calibration line and can be used to check the calibration. Use the Context Menu to switch between different display formats. You get access to this menu by clicking the right mouse button on the diagram.

Lower Diagram
This diagram shows the differences between the given and the measured values.

Double click on this double line to open the diagram in a new window. The assigned context menu is still available. Move the mouse to this double line without clicking to get the information about the statistics.

The diagram on this page shows the calibration line to check the calibration. To enlarge sections of the diagram, left click the mouse and draw a rectangle on the desired section. The section will zoom in when you release the left mouse button. Click the right mouse button to get access to the context menu. This menu contains the following menu point:

Grid
Select this option to display a grid on the diagram. This may simplify an interpretation.

Print...
Click on this command button to print the diagramm. A printer dialog will prompt you to do further settings.

Reset
Click on this command button to reset your changes.

Enable All Command Button
Click on this command button to include all standard samples in the calibration.

Disable All Command Button
Click on this command button to remove all standard samples from the calibration.

Reset Command Button
Click on this command button to undo the last calibration calculation.

Calculate Command Button
Click on this command button to calculate the mass attenuation coefficients calibration.

Corrections Command Button
Click on this command button to open the Correction Values dialog box. This dialog box is used to edit element dependent corrections.

Calibration Data Group Box
The Calibration Data Group Box contains the following elements:

Element Text Box and PTE Command Button
Select the element for which the calibration is to be conducted with this combination. Either the respective atomic number can be entered in the text box or the Select Element dialog box can be opened with the PTE command button. The command buttons Element Change can be used to increase or decrease in single steps the atomic number displayed. The name of the selected element is displayed in the display field. Only elements that have been selected as concentration elements in the deconvolution method may be selected.

Command Buttons

Click on this command button to calibrate the next element.

Click on this command button to select the standard sample in the diagram that has the next, lower given concentration.

Click on this command button to select the standard sample in the diagram that has the next, higher given concentration.

Lower Conc. [µg/g]: Text Box
Enter the lower limit for the concentration range in this text box.

Upper Conc. [µg/g]: Text Box
Enter the upper limit for the concentration range in this text box.

Calibration Weight Text Box
Enter a concentration with which the concentration of the element of interest is to be weighted before the calculation of the calibration parameters.

Color Level [%] Text Box
Enter a color level which determines the deviation of given and calculated concentrations in %. Deviations which are bigger than the entered level will be colored red.

Hide non-certified samples Check Box
Select this option to show only the standard samples with given concentration and intensity values. If this option is not selected all standard samples will be displayed.

Output Unit Check Box
Select this option to switch to a defined output unit. The default unit is ppm.

Log. Term Check Box
Mark this check box to use a logarithmic term for a Compton model during the calibration.

Comp./Ray. Ratio as Matrix Element Check Box
Mark this check box to use the Compton/Rayleigh ratio as a matrix element.

Ratio Limit Text Box
Enter a limiting value for the Compton/Rayleigh ratio in this text box. The ratio is used as a matrix beginning with this limiting value. This text box is only active if the check box described above is selected.

Compton Range Measurement Drop-down List Box
The measurement number for the backscatter region for the defined normalization region is displayed in this text box.

Compton Range Region Drop-down List Box
The region number for the backscatter region for the defined normalization region is displayed in this text box.

Calib. incl. overlapping elements Check Box
Mark this check box to do the calibration including the overlapping elements. These elements are selected via the *Overlapping Elements Command Button*.

Overlapping Elements Command Button
Click on this command button to open the Intensity Elements dialog box. All

elements that have been defined as concentration elements at the Deconvolution Page can be selected as intensity elements.

Calibration with Offset Check Box
Select this option to calibrate with an offset value.

Secondary excitation via matrix element Check Box
Select this option if you want to assign the secondary excitation to the calibration.

Matrix Elements Command Button
Click on this command button to open the Matrix Elements dialog box. All elements that have been defined as concentration elements at the Deconvolution Page can be selected as matrix elements.

K-Shell Radio Button
Select this option to switch to the K-Shell.

L-Shell Radio Button
Select this option to switch to the L-Shell.

Thick sample extrapolation Check Box
Select this option to enable the thick sample extrapolation. This is necessary if you want to measure a sample containing "heavier" elements than Fe.

Note:

Display of the calibration line and of the normalized impulse number enable you to check the calibration of the instrument and whether or not the concentrations of your samples are covered by the calibration.

During creation of user-defined methods, the diagrams allow you to check your standard samples and the quality of the calibration.

5.9 Output Page

The Output Page of the Method Window is used to do settings for the printer output. It contains the following elements.

General Group Box
The general output settings are displayed and can be changed with the dialog elements in this group box. The individual elements have the following meanings:

Drop-down List Box
Select Standard or Cement Modules depending on the selected method. When selecting cement modules, all other dialog items except the Cement Modules button will be disabled.

Base Matrix for Output Text Field
The selected base matrix for the output of the present method is displayed in this text field.

Select Button
Click on this button to select a base bond class for output. A dialog will open to choose a matrix. Bond classes can be defined in the *Configuration Editor* => Bonds.

Edit Button
Click on this button to edit the chemical bond. The Edit Chemical Bond Dialog will open to do the settings for the output bond format.

Output Unit Button
Click on this button to edit the output unit of the elements. A dialog will prompt you.

Print Form Group Box
In this group box you may choose the output form and the output destination. The group box contains the following elements.

Drop-down List Box
Choose the output form in this Drop-down list box. There are three possibilities.

- **By Sample (Elements in rows)**
  With this output form, each sample is printed on a new page, and the respective element data is printed by row in a table format. This print form allows the most adjustment.
- **By Sample (Elements in columns)**
  With this output form, each sample is printed on a new page, and the respective element data is printed in columns.
- **By Elements**
  With this output form, the printout consists of a table in which the data for all samples is sorted according to elements. This form is practical when the element data for a series of samples is to be compared. To print statistics, this selection is necessary.

Print to Printer Radio Button
Choose this option to print to a printer.

Print to File Radio Button
Choose this option to print to a file.

Print to Printer and File Radio Button
Choose this option to print to a printer and to a file.

File Settings Button
Click on this button to do special settings for the printing to a file. A dialog will prompt you to do further settings. This Button is only enabled if you select the Print to File Radio Button or the Print to Printer and File Radio Button.

Element Options Group Box
In this group box you choose which elements will be printed and the order of the elements.

Elements Button
Click on this button to open the Select Elements Dialog Box where you can choose which elements will be printed.

Sort Elements Check Box
Mark this check box if the elements by the print should be sorted with the order of elements configuration.

Order Button
Click on this button to determinate the order of elements for the printer output. The

Determinate Order of Elements Dialog Box will prompt you to do the configuration settings.

Intensity Options Group Box
Do the settings for the intensity options in this group box. The box contains the following elements.

Drop-down List Box
Select an entry of the list box.

- no counts: No intensity counts will be printed.
- net counts: The total number of intensity counts will be printed.
- normalized intensity: The normalized intensity counts will be printed.
- normalized intensity (compton): The normalized intensity counts by compton will be printed.

Show C/F for intensities
Select this option to print the "F" for fundamental calculated results.

Special Options Group Box
Do special settings in this group box. The box contains the following elements

Short Sample Header Check Box
Mark this check box if a short description of the sample (sample name, description, measurement and evaluation date) is desired, even on the first side of the sample report.

MAC Check Box
Select this option to print the ***M***ass ***A***ttenuation ***C***oefficient.

Loss of Ignition Check Box
Mark this check box if the calculated loss of ignition should also be included in the sample report.

Sum of Concentration Check Box
Select this option to print the sum of all concentrations of the elements

Overflow Calibration Range Check Box
If the calculated concentration is greater than the highest concentration in the calibration this will be marked by a "~" character if this check box is marked. This Check Box is only enabled if you select "by sample (elements in rows)" in the drop-down list box of the Print Form Group Box.

Print Statistic Check Box
Select this option to print a statistic. This check box is only enabled if you select "by elements" in the drop-down list box of the Print Form Group Box.

Cement Modules Button
Select this option to get a special printer form created for . A dialog will prompt you to do further settings assigned to the output.

See also:
Method Administration
Method Window

5.9.1 Determinate Order of Elements Dialog

Edit the order of the elements to print in this dialog. The dialog contains the following elements.

Selected Elements List Box
All elements which should be printed out are displayed in this list box.

Insert Button
Select one element in the Selected Elemtents List Box and click on this button to add this element into the Order of Output List Box.

Remove Button
Select one element in the Order of Output List Box and click on this button to remove the element of the Order of output List Box.

Delete All Button
Click on this button to remove all elements from the Order of Output List Box.

Order of Output List Box
In this list box all elements to be printed are diplayed, in order of their output.

Up Button
Select an element of the Order of Output List Box and click on this button to move it up one step in the order of output.

Down Button
Select an element of the Order of Output List Box and click on this button to move it down one step in the order of output.

OK Button
Click on this button to confirm your selection and close the dialog.

Cancel Button
Click on this button to close the dialog without changes. Your selection won´t be saved.

5.9.2 Edit Chemical Bond Dialog

This dialog is used to edit the chemical bonds you want to be displayed on the printer output. You get the following elements.

Considered Bonds Group Box
The general output settings are displayed and can be changed with the dialog elements in this group box. The individual elements have the following meanings:

Base Element
The selected element´s number is displayed in the text box. You may click on the PTE-button to open a periodic table of elements and choose another element to edit. Right of this button the name of the element is displayed. Click on the buttons right of the name of the element to step through the periodic table of elements.

Bond Notation Text Box
The bond notation is displayed in this text box. You may edit the bond notation.

Name of Bond Text Box
You may enter a name of the bond in this text box.

Conversion Factor Text Field
The conversion factor is displayed in this text field.

Bond Elements Group Box
The bond elements and the assigned stoichiometric factors are displayed and can be edited in this group box. The individual elements have the following meanings:

Element Column
In this column the selected element is displayed. Further the assigned bonds are displayed. You may edit a bond by clicking on the PTE-button which opens the periodic table of elements.

Stoichiometric Factor Column
The stoichiometric factor of the elements in the left column are displayed in this column.

OK Button
Click on this button to close the dialog and confirm the changes. The changes will be stored in the database.

Cancel Button
Click on this button to close the dialog without saving the changes.

5.10 Library of Standards Dialog Box

5.10.1 Select Standard Dialog Box

This dialog box is used to select a standard from the library of standards. This dialog box can be opened by using the *Library Of Standards* menu point in the Tools Menu of the Method Administration. The dialog box contains the following elements:

Standard Name and Description Column
The names and short descriptions of the standard samples stored in the library of standards are displayed in these columns

Dilution Column
A mark displays the use of a dilution in a standard sample.

New Command Button
Click on this command button to open the Library of Standards: Edit Standard Data dialog box in order to enter the data for a new record in the Library of standards . This command button is only active in the supervisor level.

Edit Command Button
Click on this command button to open the Library of Standards: Edit Standard Data dialog box in order to change the data for an existing record in the Library of standards . The standard sample to be changed must first be selected in the list box. This command button is only active in the supervisor level.

Delete Command Button
Click on this command button to delete the standard sample currently selected in the list box from the library of standards. This command button is only active in the supervisor level.

Display Command Button
Click on this command button to open the Library of Standards: Display Standard Data dialog box and view the data for the standard currently selected in the list box.

OK Command Button
Click on this command button to close the dialog and store the settings that have changed.

5.10.2 Library of Standards: Display Standard Data Dialog Box

This dialog box is used to display the data stored in the library of standards. The dialog box contains the following elements:

General Information Group Box

Sample Name Display Field
The name of the standard sample is displayed in this display field.

Comment Display Field
The comment of the selected standard sample is displayed in this display field.

Sample Mass (g) Display Field
The sample mass of the standard sample is displayed in this display field.

Dilution Mass (g) Display Field
The dilution material mass of standard sample is displayed in this display field.

Dilution Factor Display Field
The dilution factor calculated from the given sample mass and the given dilution material mass is automatically displayed in this display field.

Sample Specification Group Box

Average Atomic Number Calibration Check Box
This check box is marked if the selected standard sample is to be used for the Average Atomic Number Calibration.

Mass Attenuation Coefficient Calibration Check Box
This check box is marked if the selected standard sample should be used for the Mass Attenuation Coefficients Calibration.

Dilution Material Check Box
This check box is marked if the selected standard sample is to be used as a dilution material.

Settings for given conc. Group Box

Typical Unit Drop-Down List Box
The typical mass unit for entry of the given values for the standard sample. is displayed in this drop-down list box.

Sum of Conc. Display Field
The sum of the entered given concentrations is displayed in % in this display field.

Given concentration Group Box

In the Given concentration Group Box you find a table with the following columns:

First Column
The atomic number of the selected element is displayed in this column. Row 0 includes the loss of ignition .

Symbol Column
The element symbols of the selected element is displayed in this column.

Element Column
The element names of the selected element is displayed in this column.

Conc. Column
The given concentration of the selected element is displayed in this column.

Error Column
The absolute error of the given concentrations of the selected element is displayed in this column.

Level Column
The certification level for the selected element for the standard sample is displayed in this drop-down list box.

Emp. 1, 2, 3, Fund. 1, 2 and Std. Columns
These options are marked if the standard sample should be used for the calibration for the various evaluation methods for the selected element.

OK Command Button
Click on this command button to close the dialog.

5.10.3 Edit Standard Data Dialog Box

This dialog box is used to edit the data stored in the library of standards. The dialog box contains the following elements:

General Information Group Box

Sample Name Text Box
Enter a name for the standard sample in this text box. The name should be in compliance with accepted international nomenclature and may be up to 20 characters long.

Comment Display Field
The comment of the selected standard sample is displayed in this text box.

Sample Mass (g)Text Box
Enter the sample mass for the standard sample in this text box. Valid entries lie in the range between 0 and 6.5 g.

Dilution Mass (g)Text Box
Enter the dilution material mass for the standard sample in this text box. Valid entries lie in the range between 0 and 6.5 g.

Dilution Factor Display Field
The dilution factor calculated from the given sample mass and the given dilution material mass is automatically displayed in this display field.

Sample Specification Group Box

Average Atomic Number Calibration Check Box
Mark this check box if the selected standard sample is to be used for the Average Atomic Number Calibration.

Mass Attenuation Coefficient Calibration Check Box
Mark this check box if the selected standard sample should be used for the Mass Attenuation Coefficients Calibration.

Dilution Material Check Box
Mark this check box if the selected standard sample is to be used as a dilution material.

Settings for given conc. Group Box

Typical Unit Drop-Down List Box
Select the typical mass unit for entry of the given values for the standard sample.

Sum of Conc. Display Field
The sum of the entered given concentrations is displayed in % in this display field.

Given concentration Group Box

In the Given concentration Group Box you find a table with the following columns:

First Column
The atomic number of the selected element is displayed in this column. Row 0 includes the loss of ignition .

Symbol Column
The element symbols of the selected element is displayed in this column.

Element Column
The element names of the selected element is displayed in this column.

Conc. Column
Enter the given concentration of the selected element in this column.

Error Column
Enter the absolute error of the given concentrations of the selected element in this column.

Level Column
Select certification level for the selected element for the standard sample in this drop-down list box.

Emp. 1, 2, 3, Fund. 1, 2 and Std. Columns
Select this options by a left mouse click if the standard sample should be used for the calibration for the various evaluation methods for the selected element. A check mark appears in the field if the option is enabled.

OK Command Button
Click on this command button to close the dialog and store the settings that have changed.

Cancel Command Button
Click on this command button to close the dialog without storing changes to the settings.

5.11 Menu Commands

5.11.1 Commands in the File Menu

- **Method Wizard**
  Creates a new method. The X-LabPro Method Wizard will be opened to assist you.

  Toolbar:

- **Close**
  Use the *Close* command to close an opened method.

- **Print**
  Select the *Print* command to print one or more selected standard samples of the method opened in the method window. You will be promted to select a printer and do the printer settings.

  Toolbar:

- **Print Preview**
  Get a preview of the printer output of the standard sample(s) you want to print.

- **Subclass Methods**
  Select this option to sort the methods in the Tree Control. A check mark appears next to the menu item as long as the option is enabled. After enabling this option you can move the methods in the tree control via drag-and-drop. You must first close all open method windows to make use of this feature.

- **Exit**
  Use this command to end the Method Administration session. You can also use the *Close* command on the Application Control Menu.

See also:
Method Administration
Method Administration (Tree control)
Method Window
Method Administration (Toolbar)

5.11.2 Commands in the Edit Menu

- **New...**
  Use this command to create a new standard sample in the selected method. This command will open the Enter/Edit Sample Data Dialog.

- **Edit...**
  Use this command to edit a selected standard sample. This command will open the Enter/Edit Sample Data Dialog.

- **Given Concentrations...**
  Use this commands to enter given concentrations for a standard sample. This command will open the Given Concentrations Dialog Box.
- **Copy**
  This command copies the selected standard sample(s) of the present method to the X-LabPro-clipboard.

  Toolbar:
- **Paste**
  Use this command to paste standard samples from the X-LabPro-clipboard to the present method. The data of the measurements will not be pasted.

  Toolbar:
- **Paste with Data**
  Use this command to paste standard samples from the X-LabPro-clipboard to the present method. The data of the measurements will be pasted too.
- **Clone**
  This command clones the selected standard sample(s) of the present methods. This means it will copy and paste in one single step.

  Toolbar:
- **Delete**
  Use this command to delete the selected standard sample(s) from the database.

  Toolbar:
- **Define As Background...**
  Use this command to create a copy of the selected standard sample(s) and define it as background. A dialog will prompt you to choose one of six possible backgrounds.
- **Reset Measurements**
  This command resets the measurements of one or more selected standard sample(s) .
- **Reset Evaluation**
  This command resets the results of one or more selected standard sample(s) . (Sample Status will be set from A to M).
- **Import Standard Sample(s)...**
  This command imports standard samples from archive files into the selected method. A dialog will prompt you to choose one or more archive files (*.smp).
- **Export Standard Sample(s)...**
  Use this command to export and backup standard samples of the selected method. You will be prompted to choose a directory where the archive files (*.smp) will be created.
- **Evaluate...**
  Use this command to evaluate the selected standard sample(s).

Toolbar:

- **Show Spectra...**
  Shows the spectra of one or more selected standard sample(s) via the X-LabPro Spectra Viewer.
- **Results...**
  This command shows the results of a standard sample in the Display Sample Results Dialog.
- **Properties...**
  This command shows the properties of a standard sample in the Sample Properties Dialog.

See also:
Method Administration
Method Administration (Toolbar)

5.11.3 Commands in the View Menu

- **Toolbar**
  Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in the Method Administration. A check mark appears next to the menu item when the toolbar is displayed.
  See Toolbar for help on using the toolbar.
- **Status Bar**
  Use this command to display and hide the Status Bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the Status Bar is displayed.
  See Status Bar for help on using the status bar.
- **Update (Ctrl + F5)**
  Use this command to update the tree control after valid database changes have been made from X-LabPro. When using this command the tree will only be reloaded from its temporary files.
- **Rebuild**
  Use this command to update the tree control after valid database changes have been made from X-LabPro. When using this command the tree will completely re-calculated from the database. This operation will take a few seconds.
- **Update Standards List (F5)**
  Use this command to update the standards list after valid database changes have been made from X-LabPro. When using this command the standards will be reloaded from the database.

See also:
Method Administration
Method Administration (Tree Control)
Method Administration (Toolbar)

5.11.4 Commands in the Method Menu

- **New**
  Select this menupoint to create a new method. There must be opened already a method in the Method Administration, the new method will be copied from the present one. Moreover, you can select if you want to copy standards from the opened to the new method.
  Note: Background samples and dilution materials will always be copied.
- **Delete**
  Use this command to delete the opened method from the database.
- **Import...**
  Import a method from an archive file (*.mar). You will be prompted to choose the archive file.
- **Export...**
  Select this menupoint to export and backup the selected method to an archive file (*.mar). A dialog will prompt you to choose a folder where to export.
- **Create Table of Standards...**
  Select this menupoint to create a text file containing a table of all standard samples and backgrounds of the present method.
- **Adopt Defaults...**
  Select this menupoint to open the Adopt Defaults dialog box in order to adjust various settings for standard samples that have been imported or inserted into the method.

See also:
Method Administration
Method Window

5.11.5 Commands in the Tools Menu

- **Select X-LabPro Configuration...**
  Select this menupoint to define a X-LabPro configuration file (*.xcf) as your standard configuration.
- **Library Of Standards...**
  Select this menupoint to open the Library Of Standards: Select Standard dialog box. Here you may create, edit or delete standard samples.

See also:
Method Administration

5.11.6 Commands in the Window Menu

This menu is used to switch between and arrange windows. The menu is displayed in every open window. The following menupoints are available:

- **Cascade**
  Select this menupoint to arrange open windows so that the title bar of each window is visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.

- **Tile**
  Select this menupoint to arrange all of the open windows side by side so that all of them are visible. Only a portion of the other windows is displayed. Scroll within the visible portion with the scroll bars.
- **Arrange Icons**
  Select this menupoint to arrange the icons within the application window.

5.11.7 Commands in the X-LabPro Menu

The *X-LabPro* menu contains the following commands to open other applications:

- **Method Administration...**
  This command would open the Method Administration but is disabled because the Method Administration is already running.
- **Job Manager...**
  Use this command to open the Job Manager. You may also click on the button on the toolbar.
- **Routine Dialog...**
  Use this command to open the Routine Dialog. You may also click on the button on the toolbar.
- **Spectra Viewer...**
  Use this command to open the Spectra Viewer. You may also click on the button on the toolbar.
- **Configuration Editor...**
  Use this command to open the Configuration Editor.
- **Evaluation...**
  Use this command to open the Evaluation Tool.

See also:
Toolbar (Method Administration)

5.11.8 Commands in the Help Menu

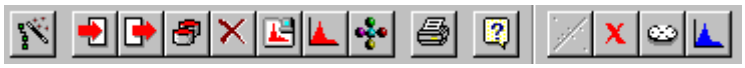
- **Contents**
  Select this menupoint to display a table of contents for the help system for the X-Lab^{Pro} program. In the help system, select the Contents command button below the menuline to show the table of contents.
- **Context Sensitive**
  Select this menupoint to open the online-help of the Method Administration.
- **Software**
  Select this menupoint to display a table of contents for the software description. Use of the operation and control software for the X-LAB energy dispersive x-ray fluorescence spectrometer is described in this section.

- **Shortcuts**
  Display the shortcuts.
- **Periodic Table**
  Select this menupoint to display the periodic table of elements.
- **About XLMethodAdmin**
  Show the version and copyrights of the Method Administration.

See also:
Method Administration
Method Administration (Toolbar)

5.12 Other

5.12.1 Toolbar



The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many functions used in the Method Administration.

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Click To

	Create a new method. The X-LabPro Method Wizard will be opened to assist you.
	Copy the selected standard(s) to the X-LabPro clipboard.
	Paste the standards from the X-LabPro clipboard to the opened method.
	Clone the selected standard(s).
	Delete the selected standard(s).
	Evaluate the selected standard(s).
	Show the spectra of the selected standard(s).
	Show the results of the selected standard.
	Print the selected standard(s).
	Show information about the application.
	Open the Method Administration.This button is disabled because the Method Administration is already running.
	Open the Job Manager.
	Open the Routine Dialog.
	Open the Spectra Viewer.

See also:
Method Administration

5.12.2 Title Bar

The title bar is located along the top of a window. It contains the name of the application and the opened method.

To move the window, drag the title bar. Note: You can also move dialog boxes by dragging their title bars.

A title bar may contain the following elements:

	Exit button.
	Maximize button.
	Minimize button.
	Name of the application.
	Name of the spectra window
	Applications icon.

6 Configuration Editor

6.1 Using the Configuration Editor

6.1.1 Menu Commands

The configuration editor XLCEdi is a module of the X-LabPro software package to configure your X-LabPro system.

Menu overview

- File Menu
- Reset Menu
- View Menu
- Help Menu
- System Menu

6.1.2 Commands in the File Menu

- **Select X-LabPro Configuration**
  Use this command to select the standard configuration, which will be load at X-LabPro start. This command will open a standard *Windows File Dialog* to select a configuration file.
- **Open**
  Use the *open* command to load an existing configuration file. This command will open a standard *Windows File Dialog* to select the configuration file.
- **Shortcuts:**

  Toolbar:

  Keyboard: CTRL+O
- **Save**
  Use this command to save the active document to its current name and directory. When you save a document for the first time, XLCedi displays the Save As dialog box so you can name your document. If you want to change the name and directory of an existing document before you save it, choose the Save As command.

Shortcuts

Toolbar:

Keys: CTRL+S

- **Save as**
  Use this command to save and name the active document. XLCedi displays the Save As dialog box so you can name your document.
- To save a document with its existing name and directory, use the Save command.
- **Print Configuration**
  Use this command to print out all configuration parameters.
- **Exit**
  Use this command to end your XLCEdi session. You can also use the *Close* command on the Application Control Menu. XLCEdi prompts you to save documents with unsaved changes.

Shortcuts

Mouse: Double click the application's Control menu Icon.

Keys: ALT+F4

6.1.3 Open Dialog Box

The following options allow you to specify which file to open:

Look in Drop-Down List Box
Select in this drop down list box the drive and the directory in which the configuration file is saved. The list will be automatically updated.

File name Text Box
Type or select with your mouse the configuration file you want to open. The list box shows all files with the extension you select in the *Files of Type* Drop-Down List Box.

Files of Type Drop-Down List Box
Select the type of file you want to open:
XCF : X-LAB^{Pro} Configuration File

Open Command Button
Click the open command button after you have selected a filename and location. The box will be automatically closed. Double clicking on a file name in the list has got the same effect.

Cancel Command Button
Close the dialog box without any activity.

Command buttons in this dialog box:

Change to the higher directory

Create a new direktory

The list shows filenames only

The list shows filenames and additional details.

6.1.4 Save As Dialog Box

This dialog box allows you to specify the name and location of the configuration file you are about to save.

Save in Drop-Down List Box
Select in this drop down list box the drive and the directory in which you want to store the configuration file. Existing files are be shown.

File name Text Box
Type a new filename to save the configuration file with a different name. XLCedi adds the extension you specify in the *Save as type* drop down list box.

Save Command Button
Click the *save* command button after you have select filename and location.This dialog box will be automatically closed. If you select an existing file name, a new dialog box will ask you to overwride the file.

Cancel Command Button
Close the dialog box without any activity.

Command buttons in this dialog box:

Change to the higher directory.

Make a new direktory.

The list shows filenames only.

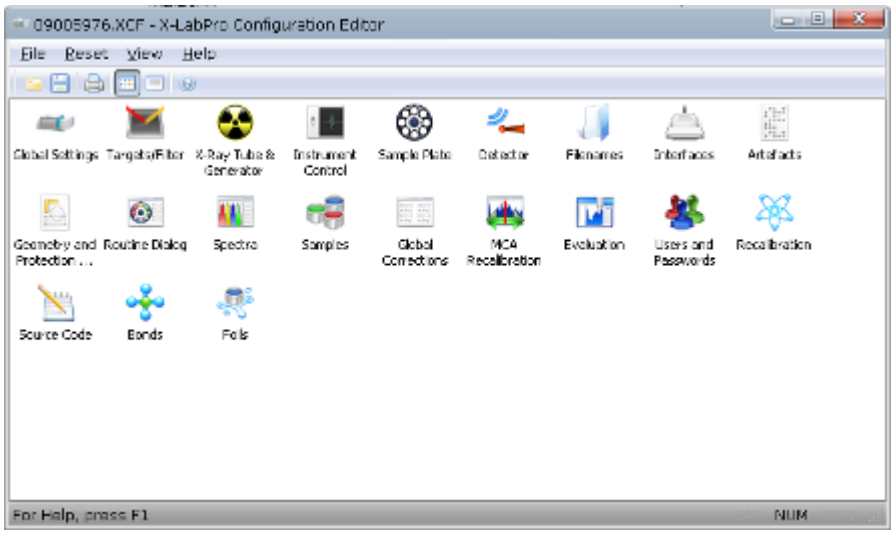
The list shows filenames and additional details.

6.1.5 Commands in the Reset Menu

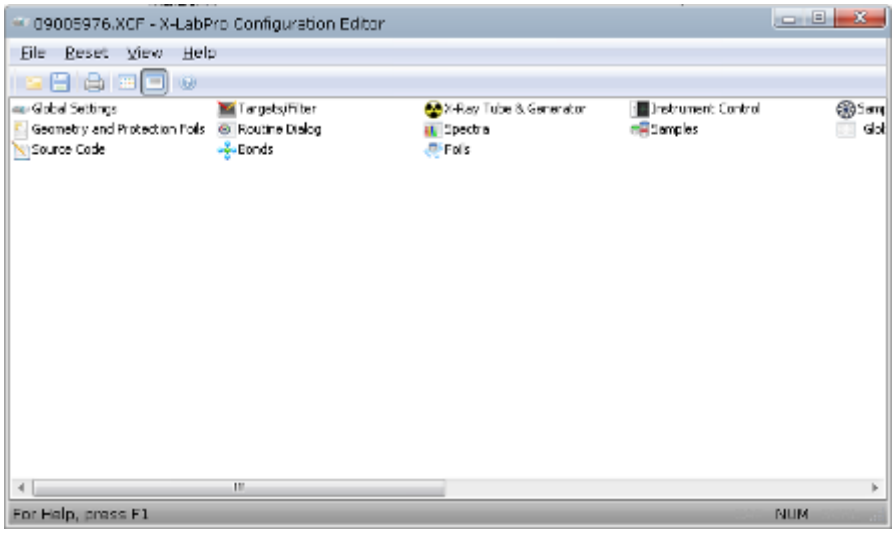
- **...to last saved**
  Resets the complete configuration to the settings in last saved version.

6.1.6 Commands in the View Menu

- **Toolbar**
  Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in XLCedi, such as File Open. A check mark appears next to the menu item when the toolbar is displayed.
- See Toolbar for help on using the toolbar.
- **Statusbar**
  Use this command to display and hide the Status Bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the Status Bar is displayed.
- See Status Bar for help on using the status bar.
- **Large Icons**
  Use this command to display the icons of the configuration editor in large icon style.



- **Small Icons**
  Use this command to display the icons of the configuration editor in small icon style.



6.1.7 Commands in the Help Menu

The *help* menu contents the following commands which will assist you by using this application:

- **Contents**
  Select this menupoint to display a table of contents for the help system for the X-LAB^{Pro} program. In the help system, select the Contents command button below the menuline to show the table of contents.
- **Context Sensitive**
  Select this menupoint to display a context sensitive help text. This menupoint corresponds to the command button with a question mark in the toolbar.
- **Software**
  Select this menupoint to display a table of contents for the software description. Use of the operation and control software for the X-LAB energy dispersive x-ray fluorescence spectrometer is described in this section.
- **Shortcuts**
  Select this menupoint to display an overview of the keyboard shortcuts.
- **About XLCedi**
  Show the version and copyrights of XLCedi.

6.1.8 Commands in the Control Menu

- **Restore**
  Use this command to return the active window to its size and position before you chose the Maximize or Minimize command.

- **Move**
  Use this command to display a four-headed arrow so you can move the active window or dialog box with the arrow keys.

Note: This command is unavailable if you maximize the window.

Size
Use this command to display a four-headed arrow so you can size the active window with the arrow keys.

After the pointer changes to the four-headed arrow:

Press one of the DIRECTION keys (left, right, up, or down arrow key) to move the pointer to the border you want to move.

Press a DIRECTION key to move the border.

Press ENTER when the window is the size you want.

Note: This command is unavailable if you maximize the window.

Shortcut
Mouse: Drag the size bars at the corners or edges of the window.

- **Minimize**
  Use this command to reduce the XLCedi window to an icon.

Shortcut
Mouse: Click the minimize icon on the title bar.

- **Maximize**
  Use this command to enlarge the active window to fill the available space.

Shortcut
Mouse: Click the maximize icon on the title bar; or double-click the title bar.

- **Close**
  Use this command to close the active window or dialog box.
- Clicking the *Close* icon and double-clicking the Control menu icon is the same as choosing the *Close* command.
- Note: If you have multiple windows open for a single document, the *Close* command on the document Control menu closes only one window at a time. You can close all windows at once with the *Close* command on the *File* menu.
- **Shortcuts**
  Keys: CTRL+F4 closes a document window

6.2 Other

6.2.1 Toolbar

The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many functions used in XLCedi.

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Click To

	Open an existing configuration file. XLCEdi displays the *Open* dialog box, in which you can locate and open the desired file.
	Save the active document or template with its current name. If you have not named the document, XLCEdi displays the *Save As* dialog box.
	Print the actually configuration.
	Switch the representation to large icon style.
	Switch the representation to small icon style.
	Display the online help.

6.2.2 Title Bar

The title bar is located along the top of a window. It contains the name of the application and document.

To move the window, drag the title bar. Note: You can also move dialog boxes by dragging their title bars.

A title bar may contain the following elements:

	Exit button
	Maximize button
	Minimize button
	Name of the document
	Applications icon. This icon shows your type of instrument or the selected dialog.

6.2.3 Status Bar

The status bar is displayed at the bottom of the XLCedi window. To display or hide the status bar, use the Status Bar command in the View menu.

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button. Moreover, during opening and closing a document, a progress bar will show you the current status.

The right areas of the status bar indicate which of the following keys are latched down:

Indicator	**Description**
CAP	The Caps Lock key is latched down.
NUM	The Num Lock key is latched down.
SCRL	The Scroll Lock key is latched down.

6.2.4 Scroll bars

Displayed at the right and bottom edges of the document window. The scroll boxes inside the scroll bars indicate your vertical and horizontal location in the document. You can use the mouse to scroll to other parts of the document.

6.3 The Configuration Editor Dialog Boxes

6.3.1 Global Settings and Instrument Data Dialog Box

This dialog box is used to edit the customer- and instrument data. This dialog box is opened with the *Global Settings* icon. The dialog box contains the following elements:

Global Settings Group Box

Customer Name Display Field
The name of the customer (your company name) is shown in this diplay field.

Instrument Number Display Field
The instrument number is shown in this diplay field.

SPECTRO Job Number Text Box
Enter the SPECTRO Job Number for the respective instrument or update in text box

Generator Serial Number Text Box
Enter the generator serial number in this text box.

Generator Serial Number Text Box
Enter the X-Ray tube serial number in this text box.

Profile Drop Down List Box and Edit Command Button Combination
Select the profile for your type of computer in this drop down list box. Click the Edit Command Button to change the timing values for your selection. In the opened Dialog Box you can change the values for following parameters

Spectrum Read Interval

Generator Read Interval

Vacuum Read Interval

Intrument Type Group Box

Intrument Type Option Buttons
Select the option button witch corresponds to your intrument type (XEPOS or SPECTRO iQ) in this selection field.

Optional Equipment Group Box (Service Mode only)

Powervar UPS
Select this check box if your intrument is equipped with an uninterruptible power supply.

Hauppauge WinTV Video System Check Box
Select this check box if your intrument is equipped with a Hauppauge WinTV Video System.

Matrox Cronos Video System Check Box
Select this check box if your intrument is equipped with a Matrox Cronos Video System.

Spectro 4.4 Data Transmission Check Box
Select this check box if you want to use the Spectro 4.4 format for the data transmission.

OK Command Button
Click on this command button to close the dialog box and store your changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.2 Targets/Filter Dialog Box

This dialog box is used to view and edit the configuration for the target drum. This dialog box is opened with the *Targets/Filter* icon. The dialog box contains the following elements:

Basic Settings Group Box

Number of Positions Drop-Down List Box
Select the number of target positions on the target drum in this drop down list box.

Valid entries are 4, 5, 6, and 8. If a number smaller than 8 is selected, the table in the Target/Filter Parameters group box is adjusted accordingly.

Changer installed Check Box
Mark this check box if your intrument is equipped with a target changer. This control is only enabled in service mode.

Always Initialize Changer Check Box
If this check box is marked, the target changer motor will be initialized before any target movement.

Offset Text Box
In this text box you can enter the offset steps that the target changer motor moves the target changer after initialisition. The unit is steps.

Target Parameters Group Box

Target Configuration Table
The configuration of the individual target positions are displayed in this table. Double click on a target position to open the *Target Position Parameters* dialog box to view a detailed description of the target position. Double clicking corresponds to the function of the *Display* command button.

Display Command Button
Select this command button to open the *Target Position Parameters* dialog box in order to view a detailed description of the currently selected target position.

Edit Command Button
Select this command button to open the *Target Position Parameters* dialog box in order to change the detailed data for the currently selected target position.

Delete Command Button
Select this command button to delete the data for the currently selected target position. This corresponds to an empty position on the target drum.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

Target Position Parameters Dialog Box

This dialog box is used to view and/or edit the detailed data for a target position. The dialog box contains the following elements:

Basic Settings Group Box

Type Drop Down List Box
Select the target type in this drop-down list box. Valid entries are: Empty, Secondary target (K), Secondary target (L), Compton/Secondary, Compton scatter, Barkla scatter and Bragg Crystal. One of the two dialog elements for a more detailed description of the target (explained below) is displayed, depending on the values selected in this drop down list box.

Name Drop Down List Box
This drop down list box is displayed when the selected target type is: Barkla scatter or Bragg Crystal. Select the name of the target in this drop down list box. Valid entries for Barkla scatter are: Boron carbide, Aluminum oxide, Beryllium, Beryllium oxide, Carbon and HOPG. The valid entry for Crystal is: HOPG.

Combination: Name Text Box, PTE Command Button and Display Field
This combination of dialog elements is displayed when the selected target type is: Compton scatter or Secondary target. The element for the target material can be chosen with this combination of dialog elements. Use either the text box to enter the atomic number or the PTE command button to select an element using the periodic table of elements. The Select Element dialog box is opened when the PTE command button is chosen. The name of the selected element is displayed in the display field.

Intensity Correction Factor Text Box
Enter the intensity correction factor in this text box. This factor can be used to make adjustments after replacing the excitation unit, for example. The factor is determined during the calibration of your instrument. Valid entries lie in the range between 0 and 2.

Primary/Secondary Diaphragm Group Boxes
These group boxes describe the primary diaphragm and the secondary diaphragm. Both group boxes have corresponding dialog elements. These are:

Material Text Box
Enter a description of the respective diaphragms material in this text box. The description can be a maximum of 20 characters long.

Inner Diameter Text Box
Enter the inner diameter of the respective diaphragm in this text box. Valid entries for the primary diaphragm lie in the range between 0 and 14 mm; in the range between 0 and 12 mm for the secondary diaphragm.

Length Text Box
Enter the length for the respective diaphragm in this text box. Valid entries for the primary diaphragm lie in the range between 0 and 10 mm; in the range between 0 and 6 mm for the secondary diaphragm.

Radiation Filter Group Boxes
These group boxes describe the filters for the target positions (Primary filter, Primary filter 2, Secondary filter 1 and Secondary filter 2). The group boxes have corresponding dialog elements. These are:

Combination: Name Text Box, PTE Command Button and Display Field
The element for the respective filter can be set with these dialog elements. Use either the text box to enter the atomic number or the PTE command button to select an element using the periodic table of elements. The *Select Element* dialog box is opened with the PTE command button. The name of the selected element is displayed in the display field.

Density Text Box
Enter the density of the filter material in this text box. Valid entries lie in the range between 0 and 25 g/cm³.

Thickness Text Box
Enter the thickness of the filter material in this text box. Valid entries lie in the range between 0 and 1000 µm.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.3 X-Ray Tube Dialog Box

This dialog box is used to view and/or edit various settings for the X-Ray tube. This dialog box is opened by clicking the *X-Ray Tube* icon.

General Information Group Box

Type Drop Down List Box
Select the type of tube used in this drop-down list box. Possible entries depent on your instrument. Entries will be automatically placed in the *Max. Power* text box and in the Characteristic Lines list box when a new type is selected in this drop down list box.

Anode Text Box
This edit control contains the atomic number of the anode material. It is possible to enter the atomic number in the edit control or to choose an atomic number from the Periodic Table of Elements by clicking the *PTE* Button.

Characteristic Lines Group Box

Grid Control for Current and Voltage for the Tube Characteristic Lines
Up to 10 pairs of current and voltage pairs, whose fit points are not components of the portion of the tube tube characteristic lines limited by the maximum power, are shown in this list box. These values are used together with the value for the x-ray tube's maximum power to check the user settings for current and voltage and to adjust them if necessary. It is possible to edit the values directly in the grid control.

Options Group Box

Generator installed Ckeck Box
Mark this check box if your instrument is equiped with a generator.

Preset Standby Mode Ckeck Box
If this check box is activated, the generator will automatically change its mode to standby mode after finishing a measurement.

Options Generator

Max. Power Text Box
Enter the maximum tube power in this text box. Valid entries lie in the range between 100 and 3000 W. This value is used together with the values for the tube characteristic lines to check the user settings for current and voltage and to adjust them if necessary. There are no possible settings that do not lie within the limits described in this dialog box.

Maximum Voltage (kV) Text Box
Enter the maximum value for the tube voltage in this text box. Valid entries lie in the range between 1 and 100 kV.

Maximum Current (mA) Text Box
Enter the maximum value for the tube current in this text box.

Delta Voltage (kV) Text Box
Enter the size of the steps with which the tube voltage should be reduced before turning off the x-ray tube. Small steps slow the reduction process; steps that are too large may lead to an error during monitoring of the relative voltage for the x-ray generator along with premature turning off of the x-ray tube. Valid entries lie in the range between 1 and 10 kV.

Delta Current (mA) Text Box
Enter the size of the steps with which the tube current should be reduced before turning off the x-ray tube. See above for further information. Valid entries lie in the range between 1 and 10 mA.

Shutter Group Box

Motor Steps Text Box
Enter the number of steps for the shutter in this text box. Valid entries lie in the range between 1 and 5000 Steps.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.4 Instrument Control Dialog Box

This dialog box is used to view and edit various instrument control settings. This dialog box is opened with the *Instrument Control* icon.

Standby Tab Control

Standby Voltage (kV) Text Box
This text box contains the generator voltage in standby mode. The unit is kV. Valid ranges depent on the selected tube and the maximum tube power.

Standby Current (mA) Text Box
This text box contains the generator current in standby mode. The unit is mA. Valid ranges depent on the selected tube and the maximum tube power.

Standby Target Drop Down List Box
In this drop down list box you can choose the target selected in standby mode.

Enable Vacuum Pump ... Check Box
If this checkbox is activated, the vacuum pump will be switched on when entering standby mode after a cuvette measurmenent. The pump time cannot be entered and is set to 5 seconds.

Vacuum Tab Control

Ventilation Time (s) Text Box
Enter the ventilation time in this text box. This is the time that is needed to ventilate the evacuated sample chamber. Valid entries lie in the range between 10 and 100 s. The sample chamber may not be completely ventilated if the value here is too small. It may, then, not be possible to open the cover for the sample chamber.

Vacuum Pump Time (s) Text Box
Enter the vacuum pump time in this text box. This is the time that is needed to produce a vacuum in the sample chamber. Valid entries lie in the range between 10 and 200 s. The sample chamber may not be completely evacuated before a measurement is started if the value here is too small; this leads to erroneous measurement values.

Postpump Time (s) Text Box
Enter the time for pumping after reaching the vacuum in this text box. This time is needed to ensure the vacuum during the whole measurement.

Vacuum Pump Installed Check Box
Mark this checkbox if your intrument is equipped with a vacuum pump.

Vacuum Measurement Installed Check Box
Mark this checkbox if your intrument is equipped with the optional vacuum measurement.

Measurement Tab Control

Optimum Dead Time (%) Text Box
Enter the optimum dead time in this text box. The calculation of the new tube current is based on this time during current regulation. If the optimum dead time cannot be achieved, despite current regulation, it is because the newly calculated current lies outside of the tube characteristic line and, thus, cannot be set. Check the excitation conditions for the measurement if this occurs.

Check Tube Cooling Check Box
If this check box is marked, the revolutions of the fan motor will be controlled. This check box is only activated for the XEPOS.

Low Energy Cutoff [eV] Text Box
Enter the low energy level (in eV) in this text box. From this level onwards events are shown in the spectral representation. This textbox is only enabled if your instrument is epuiped with a DXP.

Hide Secure Message Boxes
If this check box is marked, the secure message boxes are will be hidden.

Gas Flush Tab Control

Prepump Time (s) Textbox
Enter the prepump time in this textbox. For this time, the air in the sample room will be pumped out by the vacuum pump before the gas flush will be activated. Valid entries lie in the range between 0 and 300 s. This textbox is enabled if the *Gas Flush with Vacuum* option button is marked.

Waiting Time (s) Textbox
Enter the waiting time before the measurement in this text box. Valid entries lie in the range between 0 and 300 s. This textbox is enabled if the *Gas Flush with Vacuum* or *Gas Flush without Vacuum* option button is marked.

Minimum Gas Flow (l/h) Textbox
Enter the minimum gas flow in this textbox. Valid entries lie in the range between 0 and 1000 l/h. This textbox is enabled if the *Gas Flush without Vacuum* option button is marked.

No Gas Flush / Gas Flush with Vacuum / Gas Flush without Vacuum Option buttons
With this option buttons you are able to change between several gas flushes or no gas flush, depended on which given flushes are installed in your instrument.

Switch off gas flush Check Box
Mark this check box to switch off the gas flush during the measurement. if this check box is marked, you have to enter the gas flush times for the first and for the repeated measurements.

Permanent pumping Check Box
If this check box is marked the vacuum pump will be pumping permanent.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.5 Sample Plate Dialog Box

This dialog box is used to view and/or edit various settings for the sample plate. This dialog box is opened with the *Sample Plate* icon. The dialog box contains the following elements:

Allowed Sample Plate Sizes Group Box

List box with sample plate sizes and offsets
The possible sample plate size and the sample plate offsets for their configurations are displayed in this list box.

Insert Command Button
Click on this command button to open the *sample plate parameters* dialog box. An additional sample plate size can be inserted into the list with this dialog box.

Edit Command Button
Click on this command button to open the *sample plate parameters* dialog box. The currently selected entry in the list box can be edited with this dialog box.

Delete Command Button
Click on this command button to delete the sample plate size currently selected in the list box.

Sample Changer installed Check Box
Mark this check box if your instrument is equipped with an optionally available sample changer.

Use Correction Values Check Box
Mark this check box to enable the usage of correction values for sample plates. In the dialog box *Enter the Sample Plate Parameters* an additional command button will be visible. Click this command button to edit the correction values.

Options Group Box

Stand-By Sample Plate installed
Mark this check box if your instrument is equiped with a standby plate.

Sample Rotation Installed Check Box
Mark this check box to make sample rotation available for use.

Target by Target Option Button
In this measuring mode, the samples on the sample plate are measured according to the target. First the first measurements, then the second measurements, etc. are conducted. The first results are obtained after the complete measurement of the first sample in this measuring mode. This measuring mode enables the use of methods with different settings for the options for vacuum and gas flush for the individual measurements.

Sample by Sample Option Button
In this measuring mode, the samples on the sample plate are measured according to sample. Each sample is completely measured and then directly evaluated. The first results are obtained quicker than with the target by target mode. Only methods for which all of the settings for the vacuum and gas flush options are the same should be used together on one plate in this mode.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

Enter the Sample Plate Parameters Dialog Box

This dialogbox is used to enter or change additional settings for the sample plate.The dialog box contains following elements:

Sample Plate Parameters Group Box

Number of positions on the sample plate Text Box
Enter the number of sample position for a sample plate in this text box. Valid entries lie in the range between 0 and 40. Standard sample plates delivered with the instrument have 8, 12, 14, 18, 20 or 36 sample positionen.

Number of offset steps after initialization Text Box
Enter the number of steps that should be additionally driven to in order to correct the position after an initialization in this text box. Valid entries lie in the range between -20 und +20.

Additional Settings for Special Plate Group Box

This dialog elements will only be shown, if you mark the checkbox *Extented Sample Plate* in the *Sample Plate Parameters* Group Box.

Number of positions (32 mm)Text Box
Enter the number of 32mm positions on the sample plate in this text box.

Number of positions (40 mm)Text Box
Enter the number of 40mm positions on the sample plate in this text box.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

Correction... Command Button...
This command button is only visible if the check box *Use Correction Values* in the dialog box *Sample Plate* is marked. Click this command button to open the *position correction* dialog box. In the dialog box you can edit the correction values.

6.3.6 Detector Dialog Box

This dialog box is used to view and edit various settings for the detector. This dialog box is opened with the *Detector* icon. The dialog box contains the following elements:

Basic Settings Group Box

Type of Detector Drop-Down List Box
Select the type of the detector in this drop down list box. Possible entries depend on your instrument.

Type of Entrance Window Drop-Down List Box
Select the type of entrance window in this drop-down list box. Valid entries are: Beryllium, Boron, Diamond, Glass, Mox Tex and Siliconnitride.

Colimator
Select the type of colimator, your detector is equipt with.

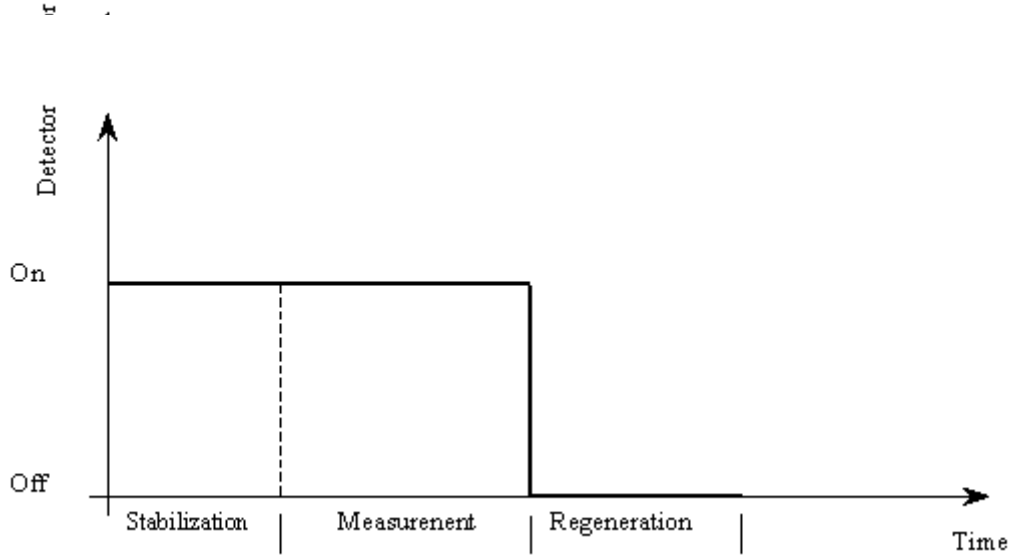
Beryllium Equivalent Thickness Text Box
Enter a value in this text box which gives the thickness of an equivalent beryllium window in regards to absorption behavior. Valid entries lie in the range between 0 and 100 µm.

Thickness Gold Contact Layer Text Box
Enter a value for the thickness of the gold contact layer in this text box. Valid entries lie in the range between 0 and 50 nm.

Thickness Silicon Dead Layer Text Box
Enter a value for the thickness of the silicon dead layer in this text box. Valid entries lie in the range between 0 and 0.5 µm.

Thickness Active Layer Text Box
Enter a value for the thickness of the active layer in this text box. Valid entries lie in the range between 0 and 5 mm.

Additional Parameters for Sirius Detectors



Activate the checkbox if you want the stabilization be started before the measurement.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.7 Filenames Dialog Box

This dialog box is used to view and enter the settings for file names for the data tables used by the program. This dialog box is opened with the *Filenames* icon. The dialogbox contains following elements:

Settings Group Box

Use Programm Directory Check Box
Mark this check box, if the data tables will be stored in the program directory of the X-LAB^{Pro} software.

Directory Text Box with Command Button
Click this command button to open the *Select Directory* dialog box. In this dialog box you can select the directory in which the data tables will be stored. Only existing directorys will be shown. Please use the windows explorer to create a new subdirectory. The text field displays the selected directory. The program directory from the X-LAB^{Pro} software is the default directory.

This dialog elements will only be visible, if the *Use Programm Directory* check box is not marked.

Database Group Box

Use DSN Name Radio Button / Drop Down List Box
Select this option if you want to use a SQL Database with X-LabPro software. In the Microsoft Windows settings you can define one or more DSN Names for SQL Databases. Select in the drop down list box the data source you want to use.

Use X-LabPro File Structure Radio Button
Select this option if you want to use the file structure as database for your X-LabPro software.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.8 Interface Dialog Box

This dialog box is used to view and edit the preset interfaces between the spectrometer and the personal computer. The parameters for the following interfaces can be set here:

Serial interface for instrument components and generator

Serial interface for detection electronics

The dialog box is opened with the *Interfaces* icon and contains the following elements:

Serial Interface Drop Down List Box
Select the serial interface to be used to control the X-Ray generator communication or the detection elektronics communication in this drop down list box.

Baudrate Drop Down List Box
In this drop down list box you can choose the baud rate for the serial communication. Typical value is 38400 for all intruments.

Serial Interface Parameters Text Box
This text box shows you the parameters for the serial interface. These parameters are baud rate, parity, data bits, stop bits and Xon/Xoff

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.9 Artefacts Dialog Box

In this dialog box parameters depending on your instument will be shown. These parameters can only be modified in service mode.

6.3.10 Geometry and Protection Foil Dialog Box

This dialog box is used to display the geometry data and to edit the parameters for the detector protection foil and the target protection foil.
This dialog box is opened with the *Geometry* icon. The dialog box contains the following elements:

Geometry Tab Control

Distance Sample ⇔ Detector [mm] Text Box
This text box displays the distance between sample and detector. This value can only be changed in service mode.

Distance Target ⇔ Sample [mm] Text Box
This text box displays the distance between target and sample. This value can only be changed in service mode.meth

Detector Protection Foil Tab Control

Foil Drop Down List Box
Select the used detector protection foil in this drop down list box.

Target Protection Foil Tab Control

Foil Drop Down List Box
Select the used target protection foil in this drop down list box .

Angles Tab Control

In this Dialog parameters depending on the used device type can be entered. These parameters should not be modified.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.11 User Dialog

6.3.12 Routine Dialog Settings Dialog Box

This dialog contains the settings for the Routine Dialog. This dialog is opens by clicking on the *Routine Dialog* icon.

Presets Tab Control

Method Class Drop Down List Box
Use this drop down list box to select the method class that is used when opening a new sample plate in the Routine Dialog.

Sample Plate Drop Down List Box
Use this drop down list box to select the type of sample plate that is used when opening a new sample plate in the Routine Dialog.

Locked Positions Drop Down List Box
Use this drop down list box to select the sample plate positions that will be locked when opening a new sample plate in the Routine Dialog. The lists of locked positions can be configured in the *Locked Positions* tab control.

Default Job Number radio buttons
With these radio buttons you can you can decide how the job name will be created automatically. You can choose between collective job as automatically used, a daily generated job (e.g. 2001_06_05), a weekly generated job (e.g. 2001_23) or a monthly generated job (e.g. 2001_06).

Open Last Sample Plate Automatically Check Box
Mark this check box if you want the Routine Dialog automatically load the last document after starting and save the current used document at closing.

Method Classes Tab Control

Insert Command Button
Click this command button to generate a new method class. You will be prompted by the *Insert Method Class* dialog box to enter the name of the new method class. After enetring the name the new method class will be added to the list.

Delete Command Button
After prompting the selected method class will be deleted.

Method Assignment Tab Control

The dialog items on this tab control can be used to assign the different methods to the method classes.

Available Methods List Box
This list box contains all methods of your X-LabPro system.

Selected Methods List Box
After selecting a method class by using the drop down list box at the top, the methods assigned to this class will be shown in the list box below.

Insert Command Button
The selected method in the left list (Available Methods) will be added to the selected method class on the right side.

Delete Command Button
After prompting a selected method in the method class (right list) will be deleted from the list.

Columns Tab Control

The columns of the Routine Dialog sample table representation can be configured by using the list on this tab control. The order of the columns can be defined and the different columns can be defined as visible or hidden.

Up Command Button
Moves the selected column in the list to the previous position. Use the Up/Down command buttons to define the order of the columns

Down Command Button
Moves the selected column in the list to the next position. Use the Up/Down command buttons to define the order of the columns.

Double Click on the Column List
By double clicking a list item the item toggles from visible to hidden.

Locked Positions Tab Control

Insert Command Button
Generates a new list of locked positions and opens the Locked Positions dialog box.

Edit Command Button
Opens the Locked Positions dialog box to edit the selected list of locked positions.

Delete Command Button
After prompting the selected list of locked positions will be deleted from the list.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.13 Locked Positions Dialog Box

This dialog is used to define the locked positions of the sample plate. After selecting the locked positions and confirming by clicking OK, the locked positions will be included in the list. This dialog is opened by clicking the buttons *Edit* or *Insert* from the group *Lists of locked positions* or by double-click on the locked positions table.

Sample plate Group Box
By clicking the positions in the sample plate of the dialog box, the position status toggles between locked/unlocked. Locked positions are displayed in dark gray and the word *Lock* will be shown in this position. Every sample plate position will be toggled (lock/unlock) by clicking into it.

Sample size Drop Down List Box
In this drop down list box, you can select the Sample Plate Size for which the settings are valid.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.14 Spectral Representation Settings Dialog Box

This dialog box is used to select the colors for the Spectra Viewer and the printer output of the spectra as well as setting the parameters for the spectral representation in the Routine Dialog. You can set the colors for the monitor and the printer independently from one another. This dialog box is opened with double click on the *Spectra* icon.

Colors for the Representation Group Box

Screen / Printer Register
In this tab you can select for which output device the various settings will be shown. You can choose between screen and printer.

Box with Sample Diagram
This box shows how the spectral representation will appear by making usage of the current settings. The example will automatically be updated by changing the settings.

Drop Down List Box
Select a component of the example in order to change the color with this drop down list box.

Red Scroll Bar and Text Box
Set the value of the color red with these dialog elements.

Blue Scroll Bar and Text Box
Set the value of the color blue with these dialog elements.

Green Scroll Bar and Text Box
Set the value of the color green with these dialog elements.

Windows Colors
Click on this command button if you want to use windows colors for the spectra representation.

Fill Spectra Check Box
Mark this check box in order to fill the areas of the spectra underneath the spectral lines. It is recommended to disable this check box for printer output.

Box with Sample Color
The appearance of the currently selected color is shown in this box.

Measurement Window Group Box
The settings made in this box affect the spectral representation during a measurement in the Routine Dialog.

Grid Check Box
Mark this check box if a grid should be displayed.

R.O.I. Check Box
Mark this check box if the *Regions Of I*nterest should be displayed.

Line Markers Check Box
Mark this check box if the line markers should be displayed. Select the line markers after activating the Select Line Markers command button.

Select Line Markers Command Button
Click on this command button to open the *Select Element* dialog box. You can select the elements for which the line markers will be displayed using the periodic table of elements in this dialog box.

Automatic Range Switch Check Box
Mark this check box if you want the range automatically switched to smaller number of channels. Enter the thresholds for the automatic range switch in the *½ Spectrum* and *¼ Spectrum* edit controls.

½ Spectrum Text Box
Enter the threshold for the automatic switch to half-spectrum-range in this text box.

¼ Spectrum Text Box
Enter the threshold for the automatic switch to quarter-spectrum-range in this text box.

First Channel Text Box
Enter the first displayed channel of the spectral representation in this test box. Valid entries lie in the range between 1 and 4031. The sum of this number and of the selected number of channels must be less than or equal to 4097.

No. of Channels Drop-Down List Box
Select the number of channels in this drop-down list box. The entries are: 64, 128, 256, 512, 1024, 2048 and 4096. See *First Channel* text box for further restrictions.

Line Cursor Text Box
Enter the position of the line curser in this text box. The entry here must lie in the range between the first channel and the last channel (first channal + number of channels -1).

X-Axis Drop-Down List Box
Select the format of the X-Axis of the spectral representation in this drop-down list box.Valid entries are: Channel Representation and Energy Representation.

Y-Axis Drop-Down List Box
Select the format of the Y-axis of the spectral representation in this drop-down list box. Valid entries are: Logarithmic Representation, Linear Representation and Square Root Representation.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.15 Select Elements Dialog Box

This dialog box is used to select several elements or the respective line markers. Click on the box for an element in order to select it. The different colors have the following meanings:

This element can be analyzed with the spectrometer. The element is not selected. Click on the element to select it.

This element can be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.

This element cannot be analyzed with the spectrometer. The element is not selected. Click on the element to select it.

This element cannot be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.

This element cannot be analyzed with the spectrometer. The element cannot be selected at this time.

This element can be analyzed with the spectrometer. However, the element cannot be selected at this time.

There is a blue triangle in the lower right corner of each box. Click on this triangle and hold the mouse key pressed; detailed information about the selected element is displayed in a dialog box.

Multiple elements can be selected in this dialog box. The current selections remain until the selection is removed from them by clicking on them.

In addition to the periodic table this dialog box contains the following elements:

OK Command Button
Click on this command button to close the dialog box and accept the current selection.

Cancel Command Button
Click on this button to close the dialog box and cancel the procedure for selecting multiple elements.

Suggest Command Button
This command button is only displayed when the dialog box is opened from the dialogs for configuration of the printout. For print functions, all of the elements between atomic number 1 and 92 can be selected. Click on this command button to select the elements that have actually been calibrated in the respective method.

K-Shell Check Box
Mark this check box if the line markers for the K-shell for the last selected element are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

L-Shell Check Box
Mark this check box if the line markers for the L-shell for the last selected element are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

M-Shell Check Box
Mark this check box if the line markers for the M-shell for the last selected element

are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

Element Text Box
Enter the atomic number for the element to be selected in this text box. Then click on the Add or Remove command button to select or remove the selection from an element.

Add Command Button
Click on this command button to add the element in the Element text box to the selection.

Remove Command Button
Click on this command button to remove the element in the Element text box from the selection.

Select All Command Button
Click on this command button to select all of the elements in the dialog box that can be selected.

Delete All Command Button
Click on this command to remove all of the elements from the selection.

Help Command Button
Click on this command button to display this help text.

See also:

Spectral Representation Settings Dialog Box
Edit Deconvolution Method Dialog Box
Special Options for Standard Printing Dialog Box
Special Options for Multi List Dialog Box
Special Options for Special (Roche) DialogBox
Tools

6.3.16 Sample Settings Dialog Box

This dialog box is used to view and edit various settings for the samples. This dialog box is opened with the *Samples* icon. The dialog box contains the following elements:

Allowed Sample States Group Box

State and Sample Table
The possible sample states including its assignment to a sample type, diameter, dilution material and the dilution factor is displayed in table.

Insert Command Button
Click on this command button to open the *Sample State* dialog box in order to insert a new sample state into this list box.

Edit Command Button
Click on this command button to open the *Sample State* dialog box in order to change the sample state currently selected in this list box.

Delete Command Button
Click on this command button to delete the sample state currently selected in the list box.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.17 Sample State Dialog Box

This dialog box is used to enter and edit a sample state and the assignment of a state to a sample type. This dialog box is opened with the *Insert* or *Edit* command button.

Sample State Name
Enter a name of the sample state in this text box.

Sample Type Drop-Down List Box
Select one of the sample type entries in order to assign your sample state to a sample type. Valid sample types are: Pressed Tablet, Melt Tablet, Liquid, Layer, Glass, Alloys, Other, Powder and Layer Thickness.

Sample Diameter Edit Field
Enter the sample diameter in mm in this edit field.

Dilution Material Drop-Down List Box
This list box contains all dilution materials from the library of standards. Select a deilution material or "-" for no dilution material here.

Sample Mass Text Box
The sample mass (in g) can be changed in this text box.

Dilution Mass Text Box
The dilution mass (in g) can be changed in this text box.

Sum/Factor Text Box
The sum of the sample mass and the dilution factor can be changed in these text boxes.

Edit sample mass and dilution mass Option Button
Select this option button in order to enter the sample and dilution masses. The total mass and dilution factor will automatically be calculated.

Edit sum of mass and dilution factor Option Button
Select this option button in order to enter the total mass and dilution factor. The sample and dilution masses will automatically be calculated.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.18 Global Corrections Dialog Box

This dialog box is used to view and edit the standardization factors determined during the global standardization. The calculation of the standardization factors is normally performed automatically when a global standardization is conducted.

Target Drop-Down List Box
Select the target from which the intensity values will be displayed in the Intensities table.

Intensities Group Box
The correction values for all elements in combination with the selected target is shown in this table. This values can be edited in the edit fields in the ”correction” column of the table.

In the both upper lines the correction factor for the coherent and the incoherent back scatter intensities from the selected target position can be entered.

In the columns *N*, *Symbol* and *Element* the atomic numbers, atomic symbols and the name of the element are displayed.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

Reset Command Button
Click on this command button to set the correction values for the selected target to the value "1".

6.3.19 MCA Recalibration Dialog Box

This dialog box is used to view and edit the settings for the detection electronics.

Selection Group Box

Peak Time and Gain Table
The possible combinations of peak time and gain are shown in this table. The values are pre-setted and depend on the used instrument and detector.

Settings Group Box

Use Settings Check Box
This check box will only be available in service mode.

Max. Energy Difference Edit Control
The value in this edit control depends on the used instrument and will only be available in service mode.

Resolution Limit Text Box
The value in this edit control depends on the used instrument and will only be available in service mode.

Zero Peak Energy Text Box
The value in this edit control depends on the used instrument and will only be available in service mode.

Optimal Target Group Box

Secondary/Compton and Barkla/Crystall Option Buttons
Select with this option buttons the best target for the selected combination of peak time and gain .

Name Drop-Down Listbox
This drop-down listbox will be shown, if you select Barkla/Crystal as optimal target. Choose a target name in this drop-down list box.

Combinations: Element Text Box, PSE Command Button and Display Field
This combination of dialog elements will be shown, if you selected Barkla/Cristal as optimal target. The element for the target material can be chosen with this combination of dialog elements. Use either the text box to enter the atomic number or the PTE command button to select an element using the periodic table of elements. The Select Element dialog box is opened when the PTE command button is chosen. The name of the selected element is displayed in the display field.

Global Group Box

Dead Time Correction Text Box
This text box will be only available in service mode.
Processing an impulse in an energy dispersive spectrometer requires a certain amount of time. During processing of the impulse, the measuring channel is blocked for additional impulses; this results in a dead time.
The impulse processing capacity, limited by this, results in dead time effects that must be taken into consideration during spectral evaluation.
In the SPECTRO X-LAB, the dead time is determined using the zero peak. The zero peak is generated by opening a gate for noise impulses at the entrance to the ADC. To do this, the amplifier input is scanned with a set clock frequency. The gate at the ADC input is only opened when there is no impulse to be measured at the time of scanning. The dead time can be calculated by comparing the number of scans with the number of processed noise impulses.
An error of < 1% results for the correction of dead times up to 70% using this method.

Min. Peak Height Text Box
The value in this edit control depends on the used instrument and will only be available in service mode.

Sigma Min. Peak Height Text Box
The value in this edit control depends on the used instrument and will only be available in service mode.

Max Energy Shift Edit Control
The value in this edit control depends on the used instrument and will only be available in service mode.

Results Group Box
The values in this text boxes represent the results of a MCA Recalibration und will be automatically updated after a new calibration.

Reset Command Button
Click on this command button, to reset the calibration constants to the standard settings.

Calibration Peaks Group Box

Number of Calibration Peaks Drop-Down List
Select the number of calibration peaks in this drop-down list box. The same number of *element* text boxes and *channel* text boxes will be editable.

Combinations: Element Text Box, PSE Command Button and Display Field
The element for the target material can be chosen with this combination of dialog elements. Use either the text box to enter the atomic number or the *PTE* command button to select an element using the periodic table of elements. The *Select Element* dialog box is opened when the PTE command button is chosen. The name of the selected element is displayed in the display field.

Channel Text Boxes
Enter the channel for the selected element in this text box.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.20 Select Elements Dialog Box

This dialog box is used to select several elements or the respective line markers. Click on the box for an element in order to select it. The different colors have the following meanings:

	This element can be analyzed with the spectrometer. The element is not selected. Click on the element to select it.
	This element can be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.
	This element cannot be analyzed with the spectrometer. The element is not selected. Click on the element to select it.
	This element cannot be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.
	This element cannot be analyzed with the spectrometer. The element cannot be selected at this time.
	This element can be analyzed with the spectrometer. However, the element cannot be selected at this time.

There is a blue triangle in the lower right corner of each box. Click on this triangle and hold the mouse key pressed; detailed information about the selected element is displayed in a dialog box.

Multiple elements can be selected in this dialog box. The current selections remain until the selection is removed from them by clicking on them.

In addition to the periodic table this dialog box contains the following elements:

OK Command Button
Click on this command button to close the dialog box and accept the current selection.

Cancel Command Button
Click on this button to close the dialog box and cancel the procedure for selecting multiple elements.

Suggest Command Button
This command button is only displayed when the dialog box is opened from the dialogs for configuration of the printout. For print functions, all of the elements between atomic number 1 and 92 can be selected. Click on this command button to select the elements that have actually been calibrated in the respective method.

K-Shell Check Box
Mark this check box if the line markers for the K-shell for the last selected element are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

L-Shell Check Box
Mark this check box if the line markers for the L-shell for the last selected element are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

M-Shell Check Box
Mark this check box if the line markers for the M-shell for the last selected element are to be displayed. The atomic number for the last selected element is displayed in the Element text box.

Element Text Box
Enter the atomic number for the element to be selected in this text box. Then click on the Add or Remove command button to select or remove the selection from an element.

Add Command Button
Click on this command button to add the element in the Element text box to the selection.

Remove Command Button
Click on this command button to remove the element in the Element text box from the selection.

Select All Command Button
Click on this command button to select all of the elements in the dialog box that can be selected.

Delete All Command Button
Click on this command to remove all of the elements from the selection.

Help Command Button
Click on this command button to display this help text.

See also:

Spectral Representation Settings Dialog Box
Edit Deconvolution Method Dialog Box
Special Options for Standard Printing Dialog Box
Special Options for Multi List Dialog Box
Special Options for Special (Roche) DialogBox
Tools

6.3.21 Evaluation Dialog Box

In this dialog box parameters depending on your instument will be shown. These parameters can only be changed in service mode.

6.3.22 Data Transmission Dialog Box

This dialog is only shown if the optionally available data transmission is activated in service mode.

Format Drop-Down List Box:
Select the used data transmission protocol in this drop-down list box.

Data Path Text Box with Command Button

You can select a directory for the automatic data storage by clicking this command button. The filename of the data can be edited in the specified method.

Transmission Program Text Box with Command Button

You can select a program sending the stored data by clicking this command button.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.23 Users and Passwords

6.3.24 User Management Dialog Box

This dialog box is used by the supervisor to manage user information. Up to 16 users with up to 4 different user levels can be entered here. The user management function enables the control of access to the analytical system when there are multiple users. The user levels can be setup so that the users assigned

to the different user levels have access only to certain functions for the analytical system. The dialog box is opened with the User management menupoint in the Tools menu. The dialog box contains the following elements:

Users must enter a username and password to use X-Lab^{Pro} Check Box
Activate this check box if you want the X-Lab^{Pro} Login dialog box to be displayed when the program is started. This enables access control to the system. If this check box is deactivated, then the user does not need to login when the program is started. The first user entered is automatically selected as the user. This user then automatically has the same access rights as a supervisor.

Allow delete only in Supervisor Mode Check Box
Activate this check box if you want that deletion of sample or spectra data is only possible in the supervisor mode. In all other modes in the job, routine and spectra window it is not possible to delete any data of measured samples.

User data List Box
A list of all of the defined users is displayed in this list box. Up to 16 users can be entered here. There must be at least one user entered and this must be in position 1. This user must be assigned to the supervisor user level even if user management is deactivated. Additional users may be defined as required.

Add Command Button
Click on this command button to open the Edit User Data dialog box for creating a new user.

Remove Command Button
Click on this command button to delete the currently selected user from the list.

Properties Command Button
Click on this command button to open the Edit User Data dialog box. The data for an entered user can be changed, or if an empty position has been selected, a new user can be entered.

Your User Data Group Box
The data for the currently logged in user is shown in this group box. This includes the login name, the complete user name and the assigned user level.

Save + OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.25 User Levels

The usage of the software contains of several user levels to do justice to the demands of the different users and if necessary to restrict the access to some functions.
Maximally 16 users can be subordinated with the following user levels:

Routine User	The routine user can only have access to the Routine Dialog, not to the main program. This is the lowest user level.
Level 3 User	The level 3 user can only have access to the routine window. He can create new amples, make measurements and analyze but not delete them. For this user level can be fixed a password but it isn´t necessary.
Level 2 User	The level 2 user can additionally to the possibilities of the level 3 user also access to the job and the spectra window. He has the possibility to delete samples and to print results in form of reports.
Level 1 User	The level 1 user has access to all windows but in the method window he can only edit non-protected samples or the ones he creates himself.
Supervisor	The supervisor has access to all windows and all options and functions. Only the from Spectro delivered methods can´t be edited by him.

6.3.26 Recalibration Dialog Box

This dialog box is used to define the sample plate settings for the different types of recalibrations. The recalibration sample plates defined in this dialog will be used as a default setting in the Routine Dialog.

When using the recalibration menu points in the Routine Dialog, the Routine Dialog will create a new sample plate document containing automatically new replicated recalibration sample data. E.g. the description of the MCA recalibration will contain more details.

Recalibration Tab Control
The type of recalibration (e.g. global recalibration, MCA, intercept recalibration, method recalibration) for which you want to define, edit or view the recalibration sample plate data can be selected here.

Sample Plate Drop Down List Box
Select the sample plate size for the selected recalibration here.

Recalibration Sample Table
The table contains a representation of the sample plate.
If you want to define a new reclibration sample on the plate, click the button in the line numbered as the sample position where you want to place the sample.
The Select Sample Dialog Box opens, pre-setted with the method you selected for the respective recalibration sample plate. Select the sample you want to place.
Note: You must select the reference samples here. New recalibration samples will automatically be created by the Routine Dialog like described above..
If you want to delete a recalibration sample from the selected recalibration plate, use the button.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.27 Bond Classes Dialog Box

This dialog box is used to view and edit bond classes. This dialog box is opened with the *Bonds* icon.

Bond Classes Tab Control
Each page of this tab control contains a defined bond class. You can add, edit or delete bond classes. The name of the page shows the name of the bond class. The table that is displayed on a page contains the chemical bond data. Click on the *edit button* in each row to open the *edit chemical bond dialog box* for editing a bond class. In this dialog you can edit the chemical bond data.

New Command Button
Click on this command button to open the *New Bond Class* dialog box. In this dialog you can enter a name for a new bond class. Use the *Use Base* check box to derive your bond class from an existing one. The new register card with the bond class name will be inserted into the tab control.

Edit Command Button
Click on this command button to open the *New Bond Class* dialog box. In this dialog you can change the name for a new bond class. The name of the tab control page will be changed.

Delete Command Button
Click on this command button to delete the currently selected bonds class. The register card will be removed from the tab control.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

6.3.28 Foils Dialog Box

This dialog box is used to view and edit the composition of different foils. This dialog box is opened with the *Foils* icon.

Foils Table
This table contains all defined foil compositions.

New Command Button
Click on this command button to open the *Edit foil* dialog box in order to insert a new foil composition.

Edit Command Button
Click on this command button to open the *Edit foil* dialog box in order to edit the current selected foil composition.

Delete Command Button
Click on this command button to open the *Edit foil* dialog box in order to delete the current selected foil composition.

OK Command Button
Click on this command button to close the dialog box and store any changes.

Cancel Command Button
Click on this command button to close the dialog box. Changes to the settings are not stored.

7 Library of Atomic Data

7.1 Using the Library of Atomic Data

7.1.1 Items of the client area

The data stored in the library of atomic data is displayed in the Library of Atomic Data. This data is used as the basis for evaluations.

The dialog box for display of the data stored in the library of atomic data is divided into the following display regions:

General Information Group Box
General information about the selected element is displayed in this group box. These parameters are: Atomic Number, Atomic mass, Name, Symbol, Melting Point, Density, Valence, electronic Structure.
It is possible to select an element directly be entering the atomic number in the atomic number edit control.

Mass Absorption Coefficient Group Box
The mass absorbtion coefficient depending on the absorbing element can be calculated in this dialog box. To calculate the mass absorbtion coefficient, edit the energy that will be absorbed and select the absorber element.

Line Energies Group Box
The line energies of the lines for the selected element are shown in a Spread table in this group box. This data is not stored for all elements. To edit the current selection in the supervisor level, click into the specific field to edit the values.

Coster-Kronig Rates Group Box
The Coster-Kronig rates for the selected element are shown in a spread table in this group box. To edit the current selection in the supervisor level, click into the specific field to edit the value.

Discontinuity Energies and Fluorescent Yields Group Box
The discontinuity energies, the discontinuity ratios and the fluorescent yields for the selected element are shown in a spread table in this group box. To edit the current selection in the supervisor level, double click into the specific field to edit the value.

Scattering Group Box
This group box contains data for scattering

Atomic Form Factor, Scatter Amplitude, Coherent and Incoherent Collision Cross Sectiones are physical values to quantify the scattering of X-rays on matter.

7.1.2 Parameters Dialog Box

This dialog box shows the polymom parameters to calculate the mass absorption coefficient. It will be opened by clicking the parameter command button and contains the following dialog elements:

Parameters to calculate the Mass Absorption Coefficient Table
In this table you can edit seleted values.

OK Command Button
Click on this command button to close the dialog box. The element displayed in the marked line of the list box will be selected.

Cancel Command Button
Click on this button to closed the dialog box and cancel the search for lines.

7.1.3 Select Element Dialog Box

This dialog box is used to select an element. Click on the box for an element in order to select it. The different colors have the following meanings:

	This element can be analyzed with the spectrometer. The element is not selected. Click on the element to select it.
	This element can be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.
	This element cannot be analyzed with the spectrometer. The element is not selected. Click on the element to select it.
	This element cannot be analyzed with the spectrometer. The element is selected. Click on the element to remove the selection.
	This element cannot be analyzed with the spectrometer. The element cannot be selected at this time.
	This element can be analyzed with the spectrometer. However, the element cannot be selected at this time.

There is a blue triangle in the lower right corner of each box. Click on this triangle and hold the mouse key pressed; detailed information about the selected element is displayed in a dialog box.

Only one element can be selected in this dialog box. A previous selection is automatically removed when a new element is selected.

In addition to the periodic table of elements, the dialog box contains the following elements:

OK Command Button
Click on this command button to close the dialog box and accept the current selection.

Cancel Command Button
Click on this button to close the dialog box and cancel the procedure for selecting an element.

Element Text Box
Enter the atomic number for the element to be selected then click on the Select command button to confirm the selection.

Select Command Button
Click on this command button to select the element displayed in the element list box or to remove the selection if it is already selected.

Help Command Button
Click on this command button to display this help text.

See also:

Library of Atomic Data Dialog Box
Target Position Parameters Dialog Box
Absorption Discontinuity Dialog Box
Average Atomic Number Calibration Dialog Box
Calibration, Compton/Empirical Dialog Box
Calibration, Fundamental Parameters Dialog Box
Select Elements (Calibration) Dialog Box
Edit Element Bonds Dialogbox
Edit Deconvolution Method Dialog Box
Edit Method Data Dialog Box
Method Development (Calibration Line)

7.1.4 Search for Element Dialog Box

This dialog box enables you to select an element whose line energies lie within a given energy range. Confirm the search to select the element in the marked line of the list box which shows you the results of the search. This dialog box is opened with the Search menupoint (Element menu) or with the button in the toolbar. The dialog box contains the following elements.

Line Energy Text Box
Enter the energy value for any lines for which you want to search in this text box. Valid entries lie in the range between 0 and 150 keV.

Search Range Text Box
Enter a value that defines the search range in this text box. All lines in the range of the line energy ± the entered value are then displayed in the list box described below.

List Box with the Located Lines
All of the lines that are stored in the library of atomic data for the selected range are displayed in this list box. Double-Click (or click the OK button) on a line in order to select the element for the XLAdLib representation.

Repeat Command Button
Click on this command button to repeat the search after making changes to the settings for the line energy or the search range. The list box with the located lines is updated.

OK Command Button
Click on this command button to close the dialog box. The element displayed in the marked line of the list box will be selected.

Cancel Command Button
Click on this button to closed the dialog box and cancel the search for lines.

7.2 Menu Commands

7.2.1 Library of atomic data

The library of atomic data XLAdLib is a new module of the X-LabPro 2.3 software package to view the atomic data. The atomic data is the basis for evaluation on your X-LabPro system.

Moreover, XLAdLib gives you the possibility to calculate the mass absorption coefficient.

Menu overview

File Menu

Element Menu

View Menu

Help Menu

7.2.2 Commands in the File Menu

Exit
Use this command to end your XLAdLib session. You can also use the Close command on the application Control menu.

Shortcuts

Mouse: Double-click the application's Control menu button.

Keys: ALT+F4

7.2.3 Commands in the Element Menu

Next
Select the next element. The atomic number will be increased.

Previous
Select the previous element. The atomic number will be decreased.

Select
Opens the Periodic Table dialog box.

Search
Opens the Search for Element dialog box.

7.2.4 Commands in the View Menu

Toolbar
Use this command to display and hide the Toolbar, which includes buttons for some of the most common commands in XLAdLib. A check mark appears next to the menu item when the toolbar is displayed.
See Toolbar for help on using the toolbar.

Statusbar
Use this command to display and hide the Status Bar, which describes the action to be executed by the selected menu item or depressed toolbar button, and keyboard latch state. A check mark appears next to the menu item when the Status Bar is displayed.
See Status Bar for help on using the status bar.

7.2.5 Commands in the Help Menu

The help menu contents the following commands which will assist you by using this application:

Contents
Select this menupoint to display a table of contents for the help system for the X-LAB^{Pro} program. In the help system, select the Contents command button below the menuline to show the table of contents.

Context Sensitive
Select this menupoint to display a context sensitive help text. This menupoint corresponds to the command button with a question mark in the toolbar.

Concept
Select this menupoint to display a table of contents for concepts. The physical and technical principles for using the X-LAB energy dispersive x-ray fluorescence spectrometer are described in this section.

Software
Select this menupoint to display a table of contents for the software description. Use of the operation and control software for the X-LAB energy dispersive x-ray fluorescence spectrometer is described in this section.

Procedures
Select this menupoint to display a table of contents for the procedures. Instructions for commonly used procedures when working with the X-LAB energy dispersive x-ray fluorescence spectrometer are given in this section.

Shortcuts
Select this menupoint to display an overview of the keyboard shortcuts.

About XLAdLib
Show the version and copyrights of XLAdLib.

7.2.6 Commands in the Control Menu

Restore
Use this command to return the active window to its size and position before you chose the Maximize or Minimize command.

Move
Use this command to display a four-headed arrow so you can move the active window or dialog box with the arrow keys.

Note: This command is unavailable if you maximize the window.

Size
Use this command to display a four-headed arrow so you can size the active window with the arrow keys.

After the pointer changes to the four-headed arrow:

Press one of the DIRECTION keys (left, right, up, or down arrow key) to move the pointer to the border you want to move.

Press a DIRECTION key to move the border.

Press ENTER when the window is the size you want.

Note: This command is unavailable if you maximize the window.

Shortcut
Mouse: Drag the size bars at the corners or edges of the window.

Minimize
Use this command to reduce the XLCedi window to an icon.

Shortcut
Mouse: Click the minimize icon on the title bar.

Maximize
Use this command to enlarge the active window to fill the available space.

Shortcut
Mouse: Click the maximize icon on the title bar; or double-click the title bar.

Close
Use this command to close the active window or dialog box.

Clicking the *Close* icon and double-clicking the Control menu icon is the same as choosing the *Close* command.

Note: If you have multiple windows open for a single document, the *Close* command on the document Control menu closes only one window at a time. You can close all windows at once with the *Close* command on the *File* menu.

Shortcuts
Keys: CTRL+F4 closes a document window

7.3 Other

7.3.1 Status Bar

The status bar is displayed at the bottom of the XLAdLib window. To display or hide the status bar, use the Status Bar command in the View menu.

The left area of the status bar describes actions of menu items as you use the arrow keys to navigate through menus. This area similarly shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button.

The right areas of the status bar indicate which of the following keys are latched down:

Indicator	Description
CAP	The Caps Lock key is latched down.
NUM	The Num Lock key is latched down.
SCRL	The Scroll Lock key is latched down.

7.3.2 Toolbar

The toolbar is displayed across the top of the application window, below the menu bar. The toolbar provides quick mouse access to many tools used in XLAdLib.

To hide or display the Toolbar, choose Toolbar from the View menu (ALT, V, T).

Click To

	Click on this toolbar button to view the information for the element with the next lower atomic number. The last element is shown again once the first element has been reached.
	Click on this toolbar button to view the information for the element with the next higher atomic number. The first element is shown again once the last element (atomic number 105) has been reached.
	Click on this command button to select an element using a representation of the periodic table of elements. The Select Element dialog box opens.
	Click on this command button to search an elementby entering a line energy range. The Search for Element dialog box opens.
	Display the online help.

7.3.3 Scroll bars

Displayed at the right and bottom edges of the document window. The scroll boxes inside the scroll bars indicate your vertical and horizontal location in the document. You can use the mouse to scroll to other parts of the document.

7.3.3.1 Title Bar

The title bar is located along the top of a window. It contains the name of the application.

To move the window, drag the title bar. Note: You can also move dialog boxes by dragging their title bars.

The Titel Bar contains the following command buttons:

	Exit command button
	Maximize command button
	Minimize command button

8 Hot Keys

In the different windows, the program offers "hot keys". These enable some of the program functions to be started directly with key combinations. The following hot keys are available:

General Hot Keys

Special Hot Keys for Method Administration

See also:

Toolbar

8.1 General Hot Keys

The hot keys that can be used in X-LabPro 5 are listed in the following table:

Key(s)	Description
F1	Display context sensitive help
F9	Activate/open Job window
F10	Activate/open the Routine Dialog
F11	Activate/open Spectra window
F12	Activate/open window for Method Development
Alt+F4	Exit Program
Alt+F12	Open dialog box with periodic table
Ctrl+F4	Close window
Ctrl+F6	Next window
Shift+F1	Display Table of Contents for Help
Delete	Delete sample(s)/sample position
Shift+Delete	Cut sample(s) and copy to clipboard
Ctrl-Insert	Copy sample(s) to clipboard
Shift-Insert	Insert sample(s) from clipboard
Shift+F5	Cascade open windows
Shift+F6	Tile open windows

See also:

Hot Keys

8.2 Job Manager Shortcuts

Shortcuts of the Job Manager window are listed in the following table:

Key(s)	Description
Ctrl+A	Mark all standard samples in the list
Ctrl+C	Copy standard sample(s) into clipboard
Ctrl+Ins	Copy standard sample(s) into clipboard
Ctrl+V	Paste standard sample(s)
Shift+Ins	Paste standard sample(s)
Ctrl+D	Paste standard sample(s) with data
Shift+Ctrl+Ins	Paste standard sample(s) with data
Del	Delete selected standard sample(s)
Ctrl+P	Print selected standard sample(s)
F1	Open the online help
F2	Edit standard sample
Ctrl+F4	Close active job window
Ctrl+Q	Close active job window
Ctrl+O	Open job
F7	Evaluate standard sample(s)
F11	Open selected standard sample(s) in the Spectra Viewer

8.3 Shortcuts

The following shortcuts can be used in the Routine Dialog:

Key	**Description**
F1	Shows help topics for the Routine Dialog.
Alt + F4	Closes the active document.
Ctrl + N	Opens a new document.
Ctrl + F6	Switches to the next document window.
Del	Deletes the selected area of the table.
Ctrl + X or Shift + Del	Cuts the selected elements from the table and adds them to the clipboard.
Ctrl + C	Copies the selected elements of the table to the clipboard.
Ctrl + V or Shift + Ins	Pastes the contents of the clipboard to the table.
Ctrl + Left Ctrl + Right	Navigate in table cell (only if activated).

8.4 Method Administration Shortcuts

Shortcuts of the Method Administration window are listed in the following table:

Key(s)	Description
Ctrl+A	Mark all standard samples in the list
Ctrl+C	Copy standard sample(s) into clipboard
Ctrl+Ins	Copy standard sample(s) into clipboard
Ctrl+V	Paste standard sample(s)
Shift+Ins	Paste standard sample(s)
Ctrl+D	Paste standard sample(s) with data
Shift+Ctrl+Ins	Paste standard sample(s) with data
Del	Delete selected standard sample(s)
Ctrl+P	Print selected standard sample(s)
F1	Open the online help
F2	Edit standard sample
Ctrl+F4	Close active method window
F5	Update standards list
Ctrl+F5	Update tree
F7	Evaluate standard sample(s)
F11	Open selected standard sample(s) in the Spectra Viewer

X-LAB^{Pro} 5 General Tutorial

9 Application guide

Additives in oil/lubricants

Application:	Check for the elements Na – Zn in oil
Sample prep.:	Pouring liquid into sample cup
Precision:	1-3 %
LOD:	Depends on elements
Quantification:	Fundamental parameters

Fuels

Application:	Check for S
Sample prep.:	Pouring liquid into sample cup
Precision:	1-3 %
LOD:	< 1 ppm
Quantification:	Fundamental parameters

Minerals/Geology/Slags/Ceramics

Application:	Check for main components
Sample prep.:	Fusions
Precision:	0.2 %
LOD:	Depends on elements
Quantification:	Fundamental parameters or alpha coefficients

Application:	Check for trace elements
Sample prep.:	Pellets
Precision:	1-10 %
LOD:	> 0.2 ppm
Quantification:	Fundamental parameters or empirical method

Metals

Application:	Analysis of metals of a defined matrix (like brass, steel...)
Sample prep.:	Polishing surface
Precision:	1-3 %
LOD:	> 100 ppm
Quantification:	Fundamental parameters

Ferro alloys

Application:	Check for main components
Sample prep.:	Pellets
Precision:	1-3 %
LOD:	> 100 ppm
Quantification:	Empirical calibration

Remark: Ferroalloys show strong particle size effects. Therefore, standards must represent the same grain size effects as the samples do.

Caused to that no international standards can be used for calibration.

Food

Application:	Na, Mg, P, Cl, K, Ca, Fe, Zn in milkpowder
Sample prep.:	Pellets, powders in sample cups
Precision:	1-5 %
LOD:	> 0.5 ppm
Quantification:	Fundamental parameters or empirical methods

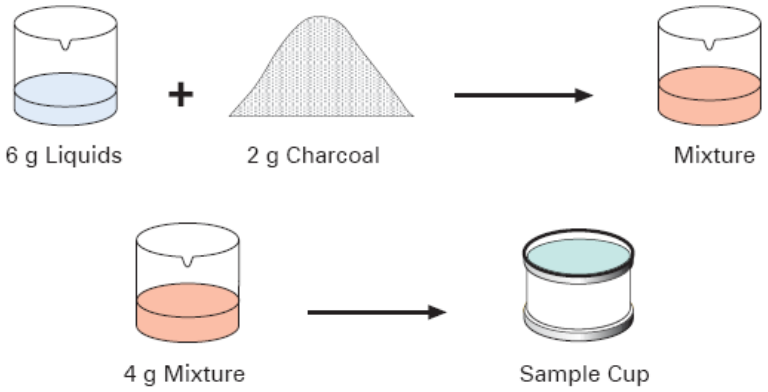
10 Sample Preparation

10.1 Sample Preparation for Liquids

If a **homogenous liquid** sample like water or oil / gasoline should be measured, it can be poured into a cuvette.

Important note:
The weights are approximated values! It is not necessary to reach exactly 4.000 g. It is sufficient to weigh between 3.8 g and 4.2 g (5 % deviation) and to enter the correct weight in the *Routine Dialog*.

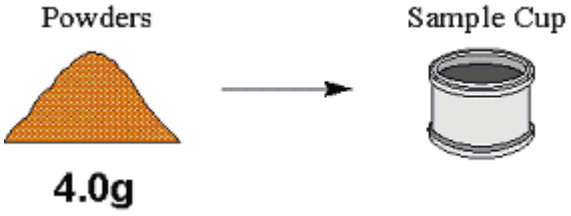
To analyze **polyphased liquids** (liquid/liquid or solid/liquid) or high volatile liquids it is recommended to use 4 g (plus-minus 5 %) of a homogenized mixture, prepared taking 6 g sample and 2 g charcoal (Merck)
(weights = plus-minus 5 %).



This mixture can be measured in the next step.

10.2 Sample Preparation for Powder Samples

Prepare a sample cup with powder.



Approx. 4 g of a powder ground down to e.g.< 63 µm is poured into a cuvette.

The bottom of the cuvette is covered by a 4 µm Prolene foil.

After pouring the powder will be slightly pressed with a pistil to form a good surface to avoid any cavities or pores at the bottom.

Important note:
The weights are approximated weights! It is not necessary to reach exactly 4.000 g.
It is sufficient to weigh between 3.8 g and 4.2 g (5 % deviation) and to enter the exact weight in the *Routine Dialog*.

10.3 Sample Preparation for Liquids / Powders

Sample type: Liquids / Powders

Additives: None

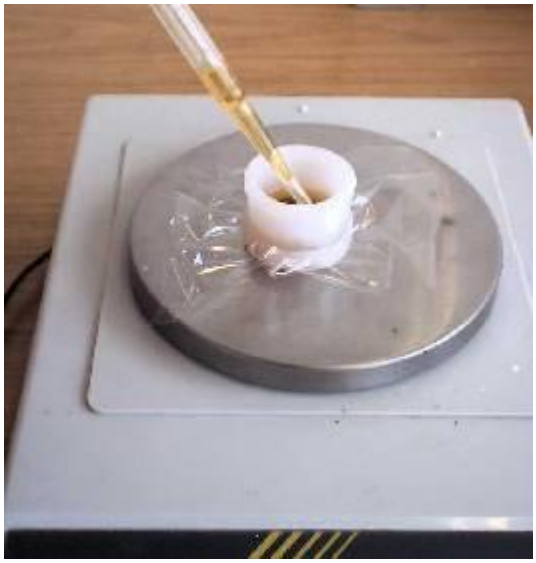
Preparation utilities: Sample cup (outer diameter 32 mm), Prolene foil (4 µm thickness)

Most sample cups are built from three parts: snap-on-ring (1), lid (2) and cell (3).

Cover cell (3) with film. Recommendation: 4µm Polypropylene film.

Click snap-on-ring (1) over the prolene foil and cell (3). Surface should be flat and smooth (no wrinkles). After placing the snap-on-ring never overstretch the foil, because this would change the thickness.

Cut foil.



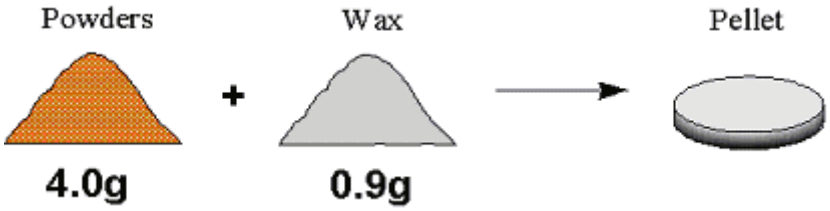
Place the sample cup on a balance. 4 g of liquid is poured into the sample cup.

Please use a weighing paper, to prevent contamination.

Close the sample cup with the lid (2). Label the sample. Leave the sample for some time (1 minute minimum is recommended) on a sheet of clean paper to check for leakage.

10.4 Sample Preparation for Pellets

The most common sample preparation for solid samples is a pressed pellet.



Approx. 4 g of a powder (e.g. < 63 µm) is homogenized with approx. 0.9 g of Hoechst Wax C and pressed to a 32 mm pellet or a 40 mm pellet.

Sample:	Powder
Additives:	Hoechst Wax C, Binder Licowax C
Preparation	Mill
Utilities:	Container for grinding and mixing
	Die (diameter 32 or 40 mm)

Important note:
The weights are approximated values (3.8 g - 4.2 g and 0.85 g - 0.95 g, respectively)! Enter the exact values in the *Routine Dialog*.

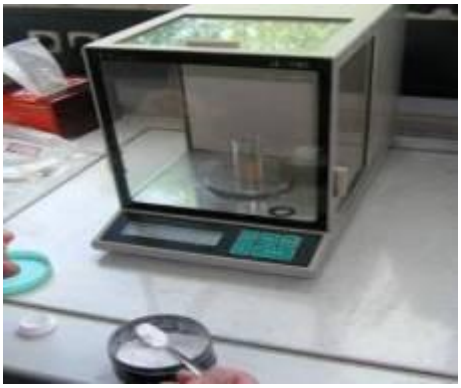
10.5 Preparation of Pressed Powder Pellets in Rings

Some powders may require pressing to insure that the bulk density of the samples is reproducible. If elements like Na and Mg need to be analyzed with highest sensitivity, the powdered samples need to be prepared as pressed pellets or as fused beads.

In case of a pressed pellet the powder can either be pressed directly or a binding material is added.

To achieve highest stability of the pressed pellets and to get best possible precision of the sample preparation procedure it is recommended to press the samples into 40 mm (1.57”) steel rings.

Weigh 5 (± 0.1) g of pulverized sample material (optimum grain size < 60 µm) into a mixing beaker and add 1 (±0.05) g of binder Clariant Licowax C (HWC). Note all weighs because these have to be entered into the software when analysing the sample.



Add two Polyamide balls (diameter 7-10 mm) into the mixing vessel.

Use a blender or mixer mill at 40- 60 % speed for 3 (±0.5) minutes to create a homogeneous mixture.

Prepare all parts of the die and make sure, that all parts are clean and dry.

Put the outer part of the die on the bottom part of the die.

Press the outer part down as much as possible.

Insert of the pressing plate (shining side to the top) into the die and make sure that this has moved to the bottom of the inner hole.

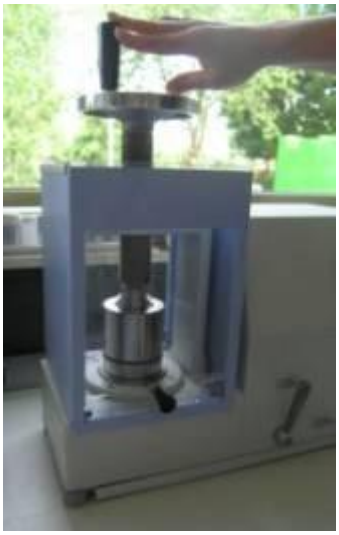
Insert a reusable steel ring into the die and make sure, that this has moved to the top of the pressing plate.

Insert the longer steel-tube into the die and onto the steel ring.

Remove the two Polyamide balls out of the mixing beaker.

Fill the sample-mixture carefully into the die and make sure, that a relatively plane surface is achieved on the top side.

Hold the steel tube with two fingers and insert the pressing cylinder into the die carefully.



Put the die into a press and press the content into a pellet at a pressure of 10 - 25 t.

Hold the pressure for 20 - 30 s.

Release the pressure and remove the die from the press.

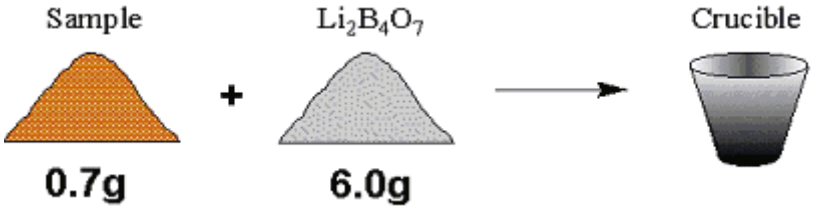
Remove the bottom of the die and press the die to the table as long as the pressing plate and the sample steel ring become visible.

Remove the pressing plate, the steel ring with the pressed pellet.

Take out the steel tube and the pressing cylinder as well.
Clean all parts of the die carefully else with Iso-Propanol or a mixture of cleaning agent.
Dry all parts carefully after cleaning and store them in a dry, dust-free environment.

Place the pressed pellet with the steel ring on the precision sample tray.
The combination of this sample preparation technique together with the precision plate offers the highest grade of stable, reproducible sample preparation for pressed pellets with highest accuracy of sample positioning in the analyzer.

10.6 Sample Preparation for Fused Beads



After the mixture is prepared and possible additives like nitrates for preoxidations were added prepare a bead as shown in the following picture.

Sample:	Powder
Additives:	Lithiumtetraborate or other borates, wetting agent
Preparation Utilities:	Platinum/Gold crucible and mould
	Fusion machine or furnace

The sample material must be dried and milled to a grain size below e.g. 63 µm.

Approx. 0.7 g of the powder is homogenized with around 6.0 g of Lithiumtetraborate and then fused at 1100 °C to form a bead. As standard procedure 10 minutes fusion time should be sufficient.
Depending on the material and the fusion machine time and temperature may vary.
Also, for some materials a preoxidation can be necessary. Especially Sulfur present in sulfidic form is very sensitive against too high temperatures and it tends to evaporate. To avoid this, a preoxidation (for example with Nitrates) can help.
Another possibility is the use of different borate like Tetraborate-Metaborate-Mixture, which melts at around 950 °C.

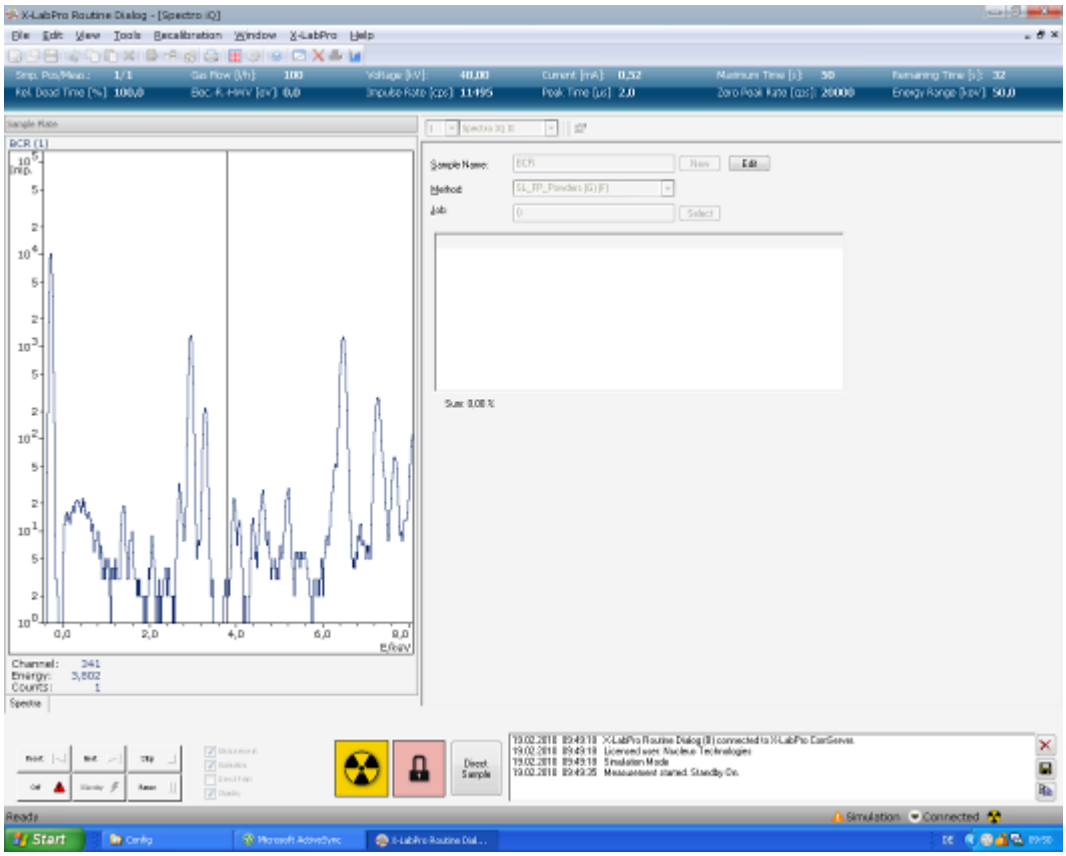
In some cases it is obligatory to reduce the sample amount down to 0.2 g. If a lot of fusion remains in the crucible the use of a wetting agent (e.g. NH_4I) can be necessary.

Note: There are some materials which may destroy your Pt/Au crucible.
The most dangerous ones are all kind of metals, especially elemental silicon, boron or iron.
Also, carbides are dangerous.

Important note:
The weights are approximated values! It is not necessary to reach exactly 0.70 g and 6.00 g, respectively.
It is enough to weigh between 0.65 g and 0.75 g (5 % deviation) and 5.7 g - 6.3 g, respectively, and to enter the exact weight in the *Routine Dialog*.

11 Measuring a sample - The Routine Dialog

All measurements are initialized from the *routine dialog*. To open the *Routine Dialog* select the following symbol in the icon bar or use the X-LabPro Communication Server.



As an example the foregoing picture shows the *Routine Dialog* for the SPECTRO iQII comprising three different parts:

- The left part of the screen shows either a spectum.

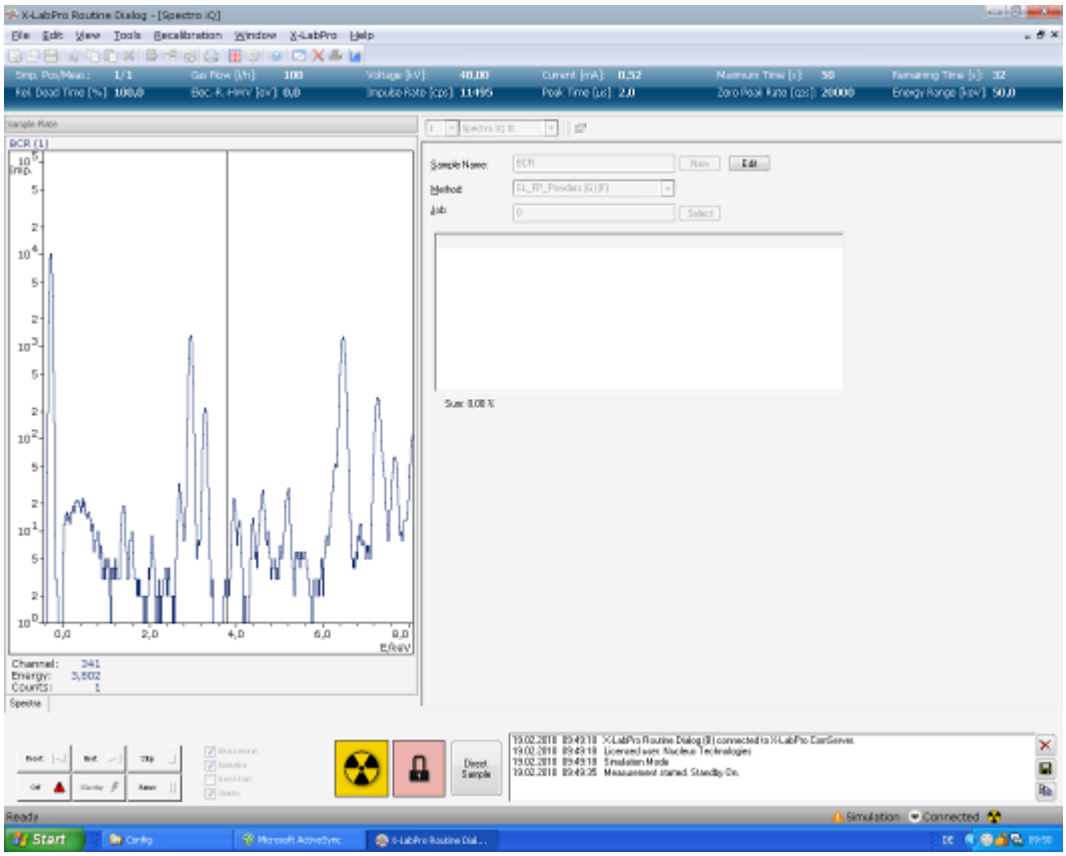
- The right part shows a table presenting the results of the measured sample or, as shown in the screenshot above, the sample plate as spreadsheet.

- The bottom part shows the control buttons to start or stop the measurement and a presentation of the actual logfile.

To configure the *Routine Dialog,* use the section *Routine Dialog* in the Configuration Editor.

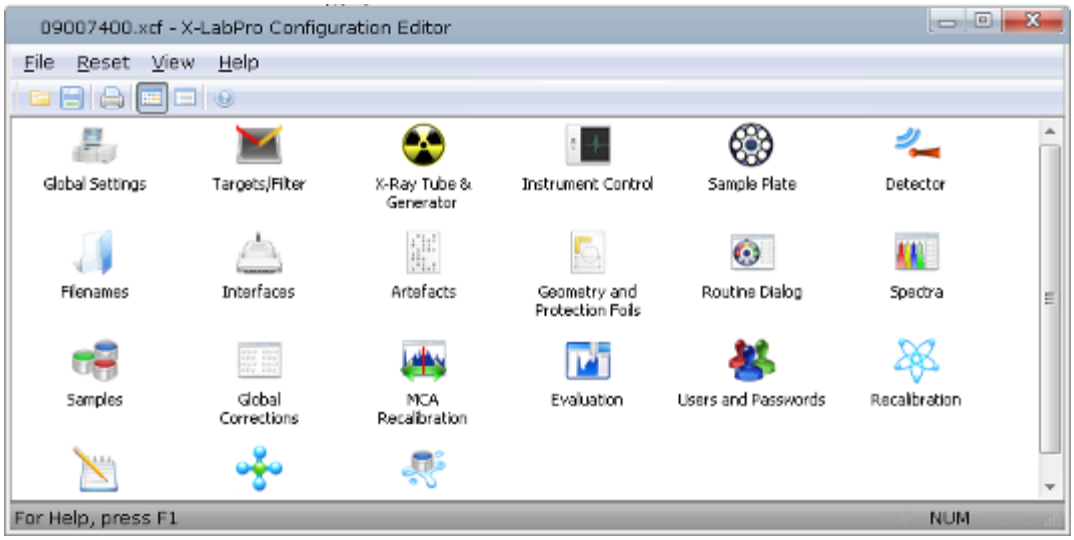
11.1 Configure Routine Dialog

The Routine Diakog is the user interface to use the X-Lab[Pro] software for daily work.



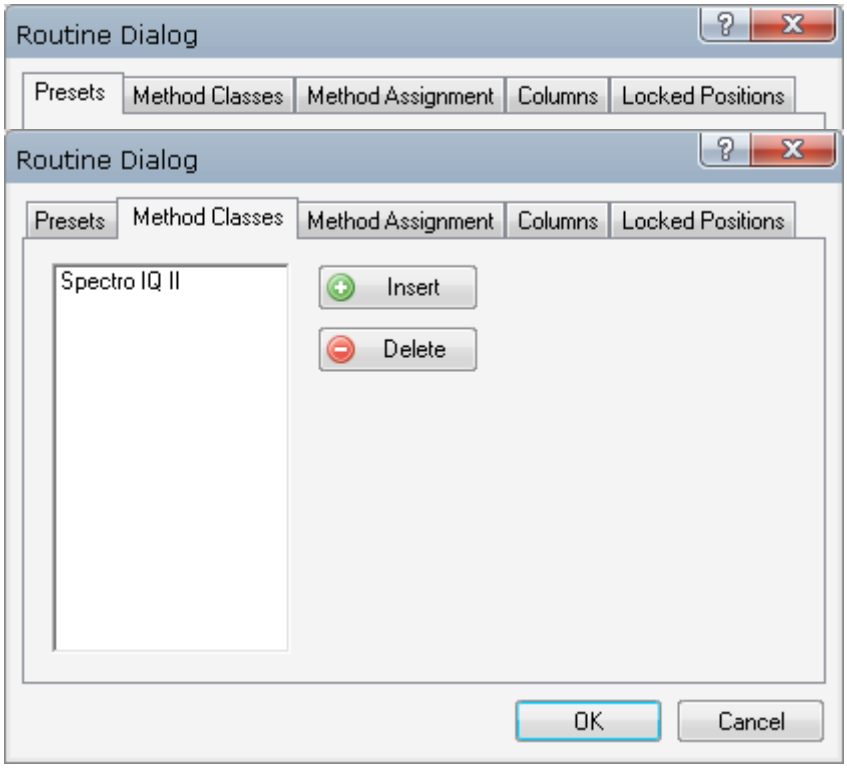
The configuration of the *Routine Dialog* is handled from the *Configuration Editor*.

Start the Configuration Editor from the X-LabPro Communication Server.

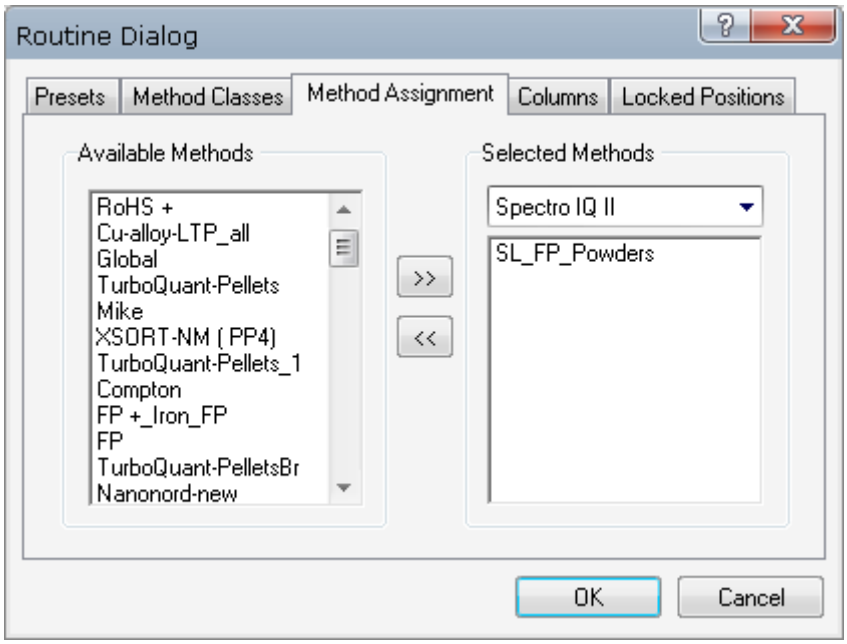


If a Supervisor is logged-in, the settings for the *Routine Dialog* can be reached with the corresponding icon.

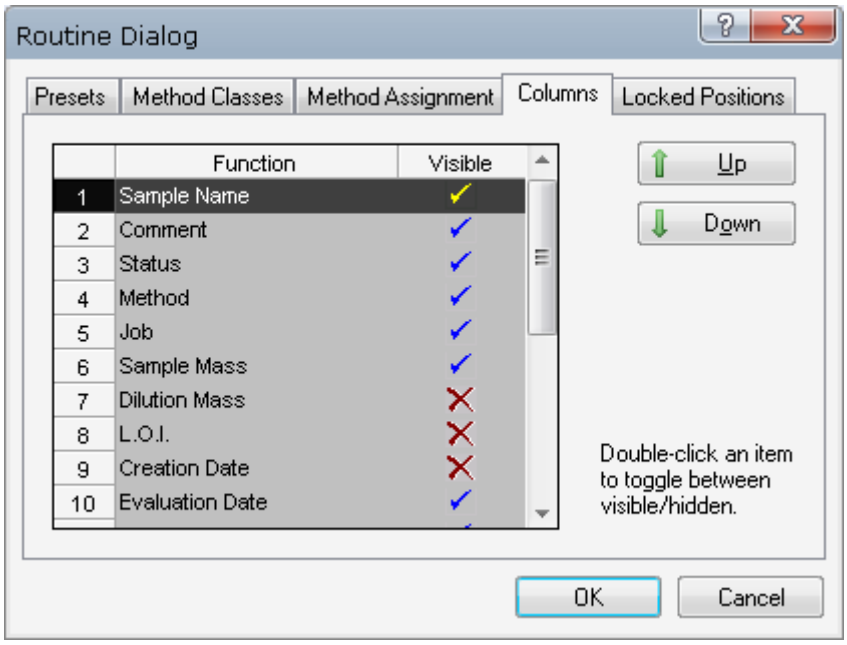
The first tab (*Presets*) allows to define some parameters like:
- Preset Method Class
- Sample Plate (number of samples - if available)
- Locked Positions (of a sample tray)
- The suggested Job Name (Job Number)



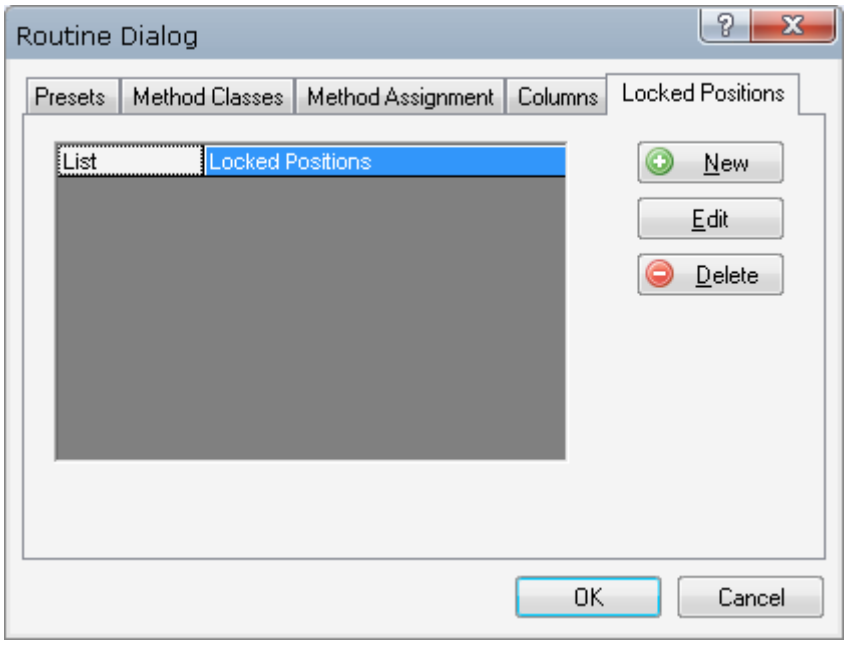
A method can be assigned to a method class (third tab).
That's an important step, because **only methods belong to a method class can be used in *Routine Dialog*!**



For other instruments, which use a table instead of the result screen, the *Columns* can be selected:

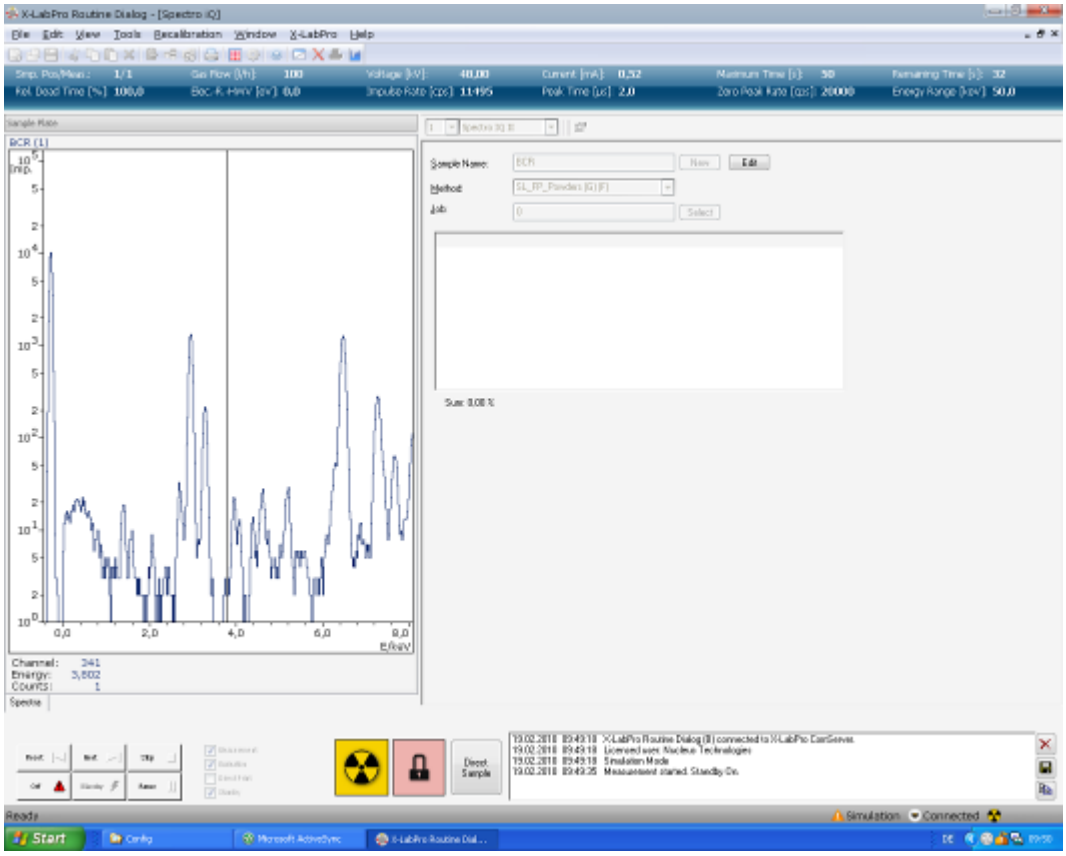


On a sample tray some positions can be locked (right tab).
This can be done to ensure that no liquid sample in position 1 can be forgotten in the instrument.



11.2 Routine Dialog

All measurements are initialized from the *Routine Dialog*.
To open the *Routine Dialog* select the following symbol in the icon bar or use the X-LabPro Communication Server.



As described before, the *Routine Dialog* comprises three different parts:

- At the left the presentation of the spectra of the actual measurement is shown.
- The right part shows the sample information.
- At the bottom the control buttons to start or stop the measurement are placed, together with a presentation of the actual logfile.

To create a new sample define a sample name and a related job name and select a method.

Normally, all settings (like available methods) are defined in the right way. Whether a job can be selected depends on the configuration of the software, because there are different options:
A job name will be created automatically by the software (e.g. the actual week) or the name of the job can be edited.

If a method is missing, please ask your supervisor to adjust it, using the Configuration Editor.

Each sample needs a *name*, a *method* and a *job* as a description. The *name* does not have to be unique but it should help identifying the samples. By selecting a *method* the measurement conditions and the sample type are preset to the default settings of this *method*. To change the selected *Method* or *Job* use the respective drop-down menu.

Jobs are the different sub-directories for your database. Similar to folders on your hard disk they help you to organize your measurements.

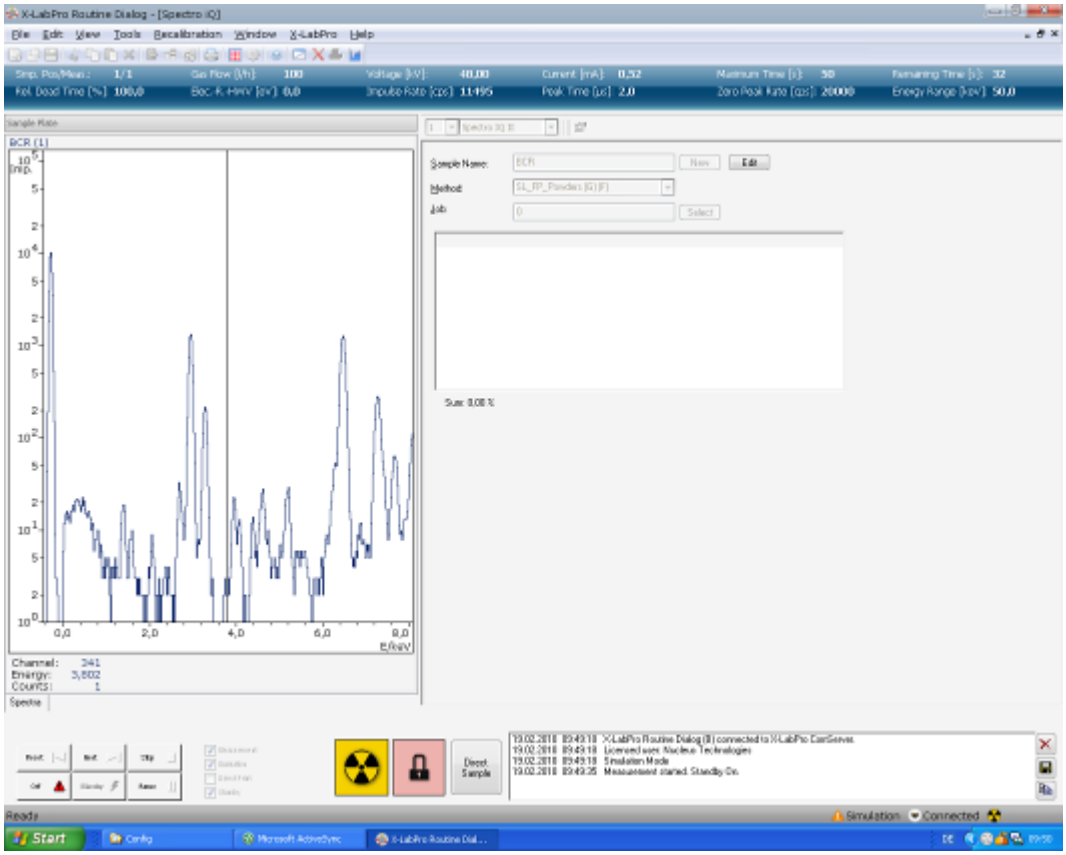
By selecting a method the default values of the *Method* will be displayed. The details like sample weightes and diameter can be edited if needed.

Now it is possible to create additional samples on different positions or to start the measurement. To start the measurement click *Start*.

Depending on the selected method, the samples will be measured in vacuum, with gas flush or in air. Whenever the samples shall be measured either with vacuum or gas flush a warning message will pop up on the screen to inform you about this measurement condition. **Never run liquids in vacuum to prevent harm to your instrument.** If you are sure about the measurement conditions confirm with *Yes* and the measurement will begin. Selecting *No* will cancel the entire measurement.

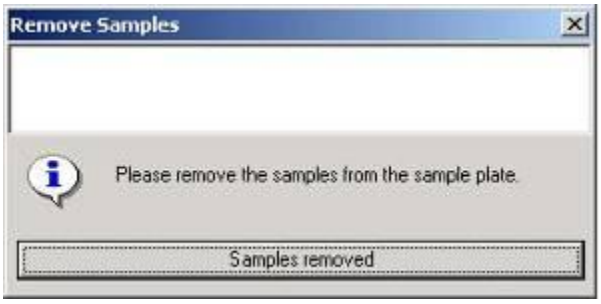
An additional message will inform about a protection foil, if the last one is defined in the selected method.

While the measurement is running, the screen looks like the following one.



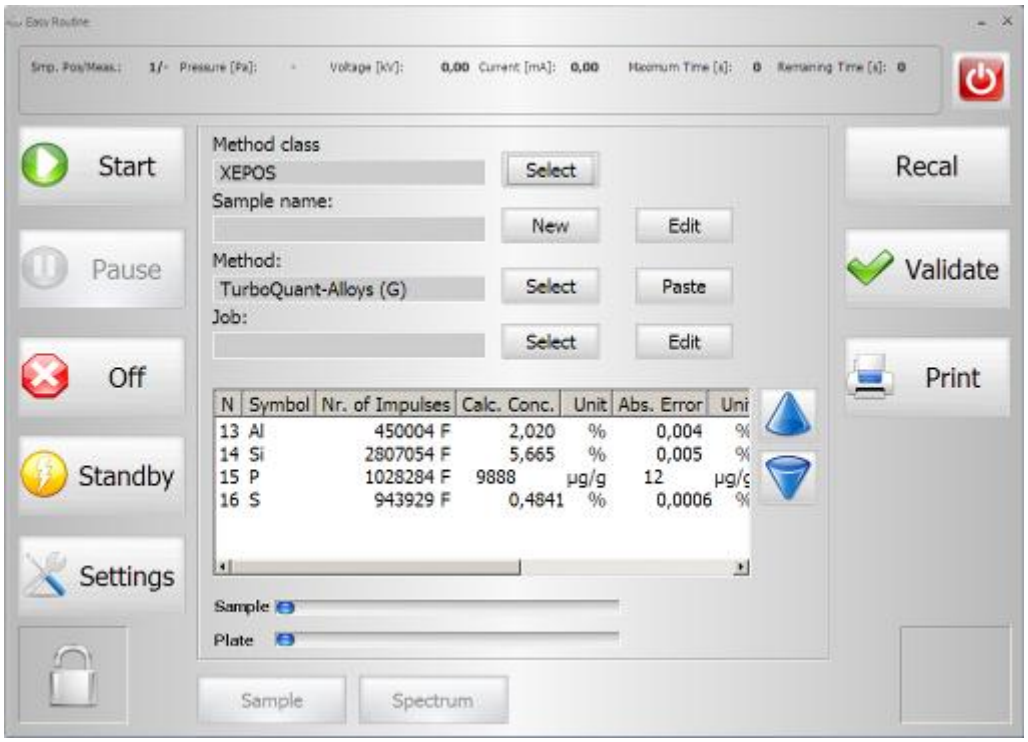
It is possible to use the Spectra Viewer Tool-Box, e.g. to identify peaks in the spectrum.

At the end of the measurement (depending, whether a sample cup for liquids or powders was used or not), an additional message will appear:



After the measurement is completed, the results will be shown (two pictures above). To start a new measurement, use *New* (right side of the sample name) or paste the sample from Job/Method using the clipboard.

The SPECTRO iQ also allows the use of a Easy user interface, which is even easier to handle:



Simulation Mode

There are two situations, when software starts the *Simulation Mode:*
1. If no instrument could be detected (Instrument off or not connected)
2. If the Simulation Mode ist selected manually.

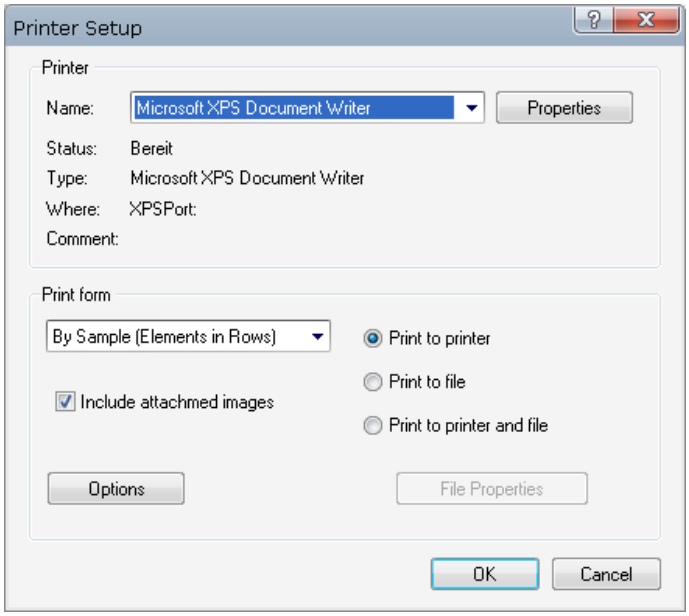
The *Simulation Mode* allows to simulate a measurement without an instrument (e.g. on exhibitions). Doing this a set of stored spectra will grow in the Routine Dialog and it looks like a real measurement. Please note that these spectra are just simulated and do not show the samples placed into the instrument. Therefore, a messagebox will inform you during the start of the Routine Dialog, if the *Simulation Mode* is activated.

12 Printing results

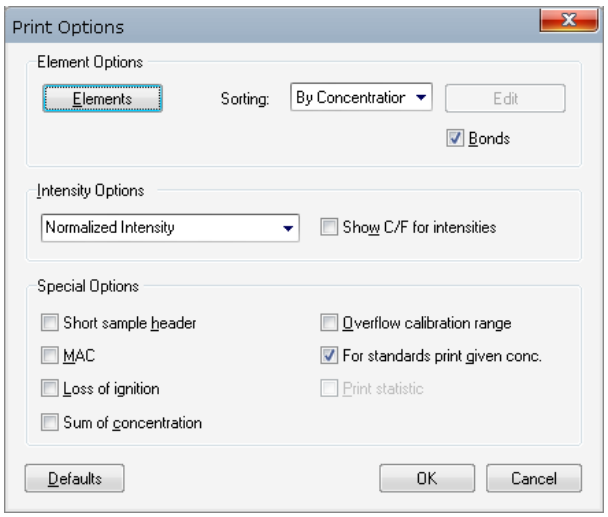
The layout of the output is defined in the *method*.

To print results select the *Print...* option from the pull-down menu *File* or select the printer symbol in the icon bar or enable the *Direct Print* option in the lower left part of Routine.

Various printing options can be selected as shown in the screen below.



In the same window it is possible to change the layout for the selected print job. Modifications will not affect the default settings of the *method*.

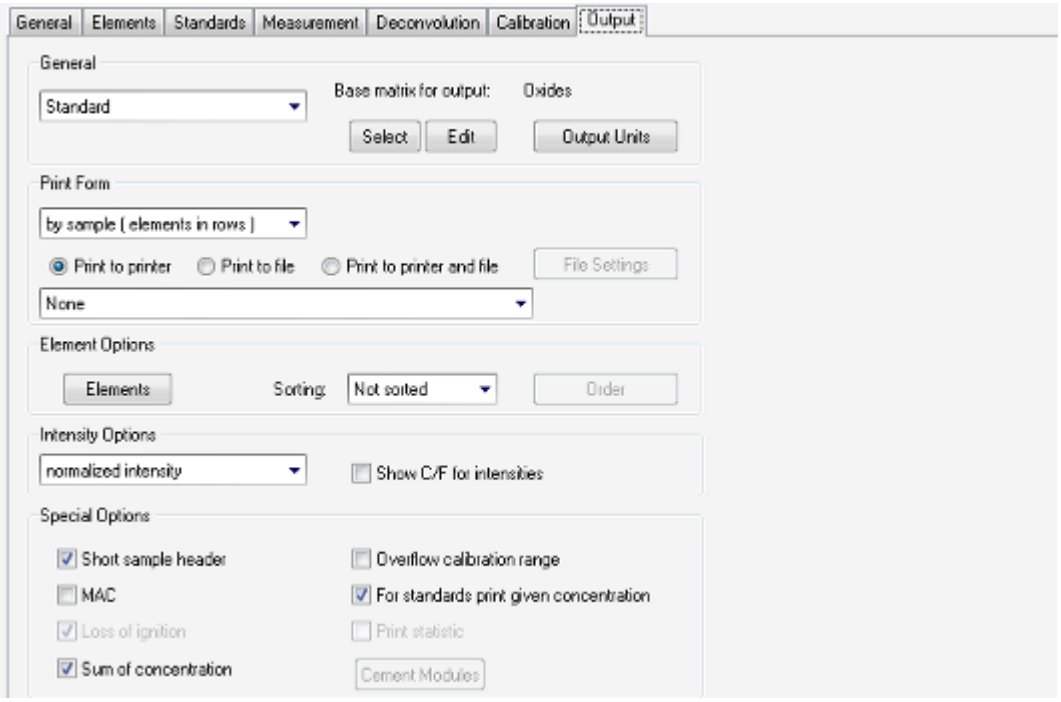


To get a first impression, it is possible to display a preview before printing by selecting Print Preview in the *file* pull-down menu.

12.1 Output

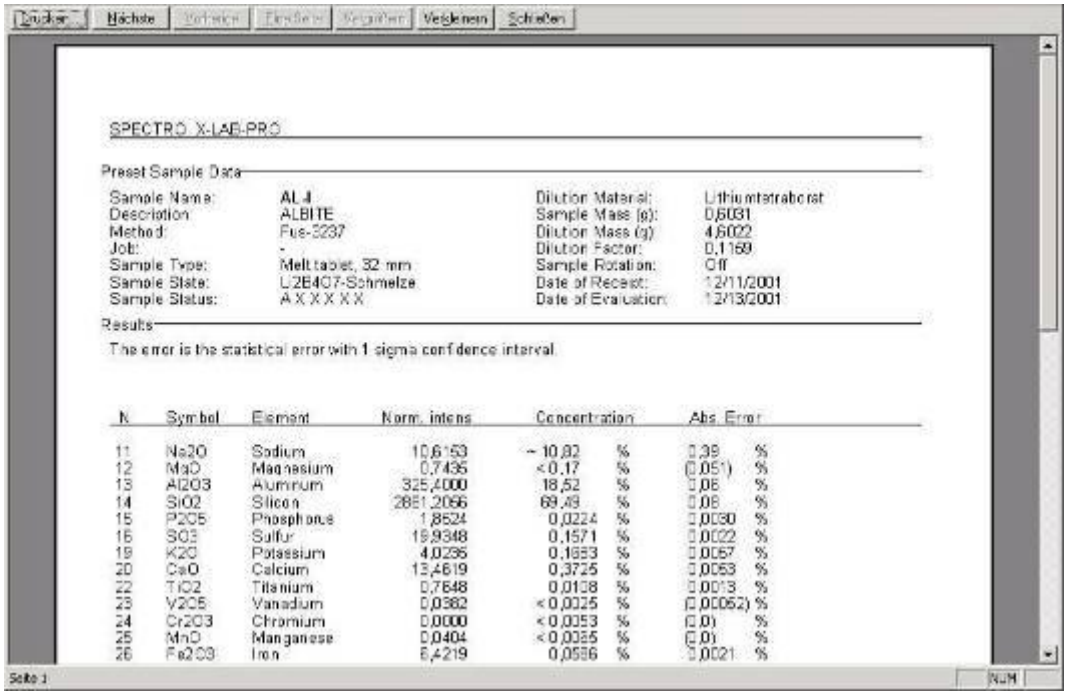
The tab *Output* is used to select the elements~~,~~ which should be printed / shown on the screen.

In addition, that's the place to define, whether bonds should be used, whether the elements should have a special *Order*, and to select the *Output Units* for each element separately.



12.2 Print Preview

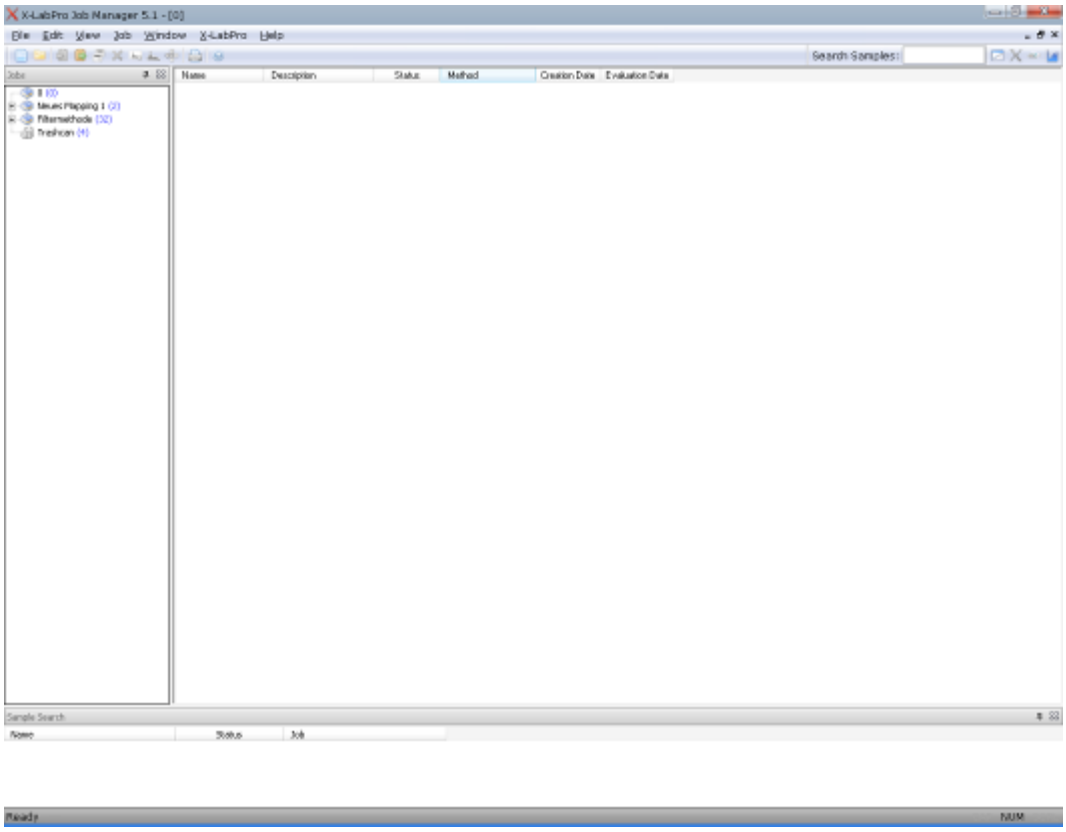
The feature Print Preview as part of the file menu allows getting an impression of the printout before printing.


Drucken...
Nächste
Vorherige
Einstellen
Ausgeben
Verkleinern
Schließen
SPECTRO X-LAB-PRO
Preset Sample Data
Sample Name: AL4
Description: ALBITE
Method: Fus-3237
Job: -
Sample Type: Melt tablet, 32 mm
Sample Siste: Li2B4O7-Schmelze
Sample Status: A X X X X X
Dilution Material: Lithiumtetraborat
Sample Mass (g): 0,6031
Dilution Mass (g): 4,6022
Dilution Factor: 0,1159
Sample Rotation: Off
Date of Receipt: 12/11/2001
Date of Evaluation: 12/13/2001
Results
The error is the statistical error with 1 sigma confidence interval.
N Symbol Element Norm. intens Concentration Abs. Error
11 Na2O Sodium 10,6153 ~ 10,82 % 0,39 %
12 MgO Magnesium 0,7495 < 0,17 % (0,051) %
13 Al2O3 Aumrum 325,4000 18,52 % 0,06 %
14 SiO2 Silicon 2851,2066 69,49 % 0,08 %
15 P2O5 Phosphorus 1,8524 0,0224 % 0,0030 %
16 SO3 Sulfur 19,9348 0,1571 % 0,0022 %
19 K2O Potassium 4,0236 0,1883 % 0,0057 %
20 CaO Calcium 13,4619 0,3725 % 0,0053 %
22 TiO2 Titanium 0,7648 0,0108 % 0,0013 %
23 V2O5 Vanadium 0,0382 < 0,0025 % (0,00052) %
24 Cr2O3 Chromium 0,0000 < 0,0053 % (0,01) %
25 MnO Manganese 0,0404 < 0,0085 % (0,01) %
26 Fe2O3 Iron 6,4219 0,0586 % 0,0021 %
Seite 1
NUM

13 Working with jobs

The Job Manager is a tool to organize the measured samples. The jobs are comparable to subdirectories or folders. In each job the software can handle up to 1000 samples. How to sort the samples in different jobs is up to the user.

To work with jobs select the *Job Manager*... option from the *X-Lab*^{Pro} menu.

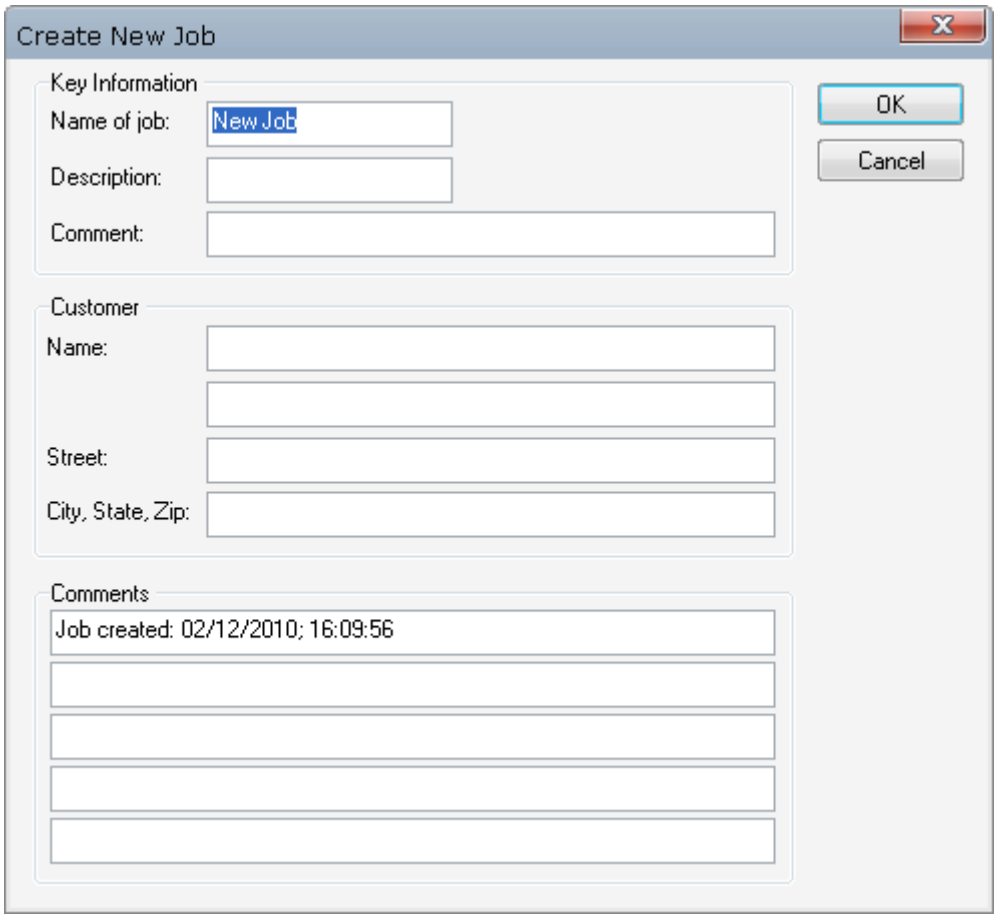


In the left part, all available jobs are shown and you have access to the general information for each job.

At the right side, a list of all samples in the selected job is shown.

To create a new job select the *New*... button in the *Job* menu.

Whenever a new job is created, a window will pop up to edit the name and other information for the new job.



As default entries for the new job the settings of the job selected before will be used as template.
Change the *Name of Job* to the desired new name.

In addition to the *Name of Job* and *Description,* further information can be edited. This additional information might be the address of a customer (especially if only samples for a specific customer are stored in a specific job) and a comment. If you select the *coversheet* option in the print options dialogue the coversheet will contain this information.

Confirm the settings of the new job by selecting the *OK* button.

14 The Recycle Bin

An additional feature in X-LabPro is the Recycle Bin. It allows to "undelete" samples, which were erased before.

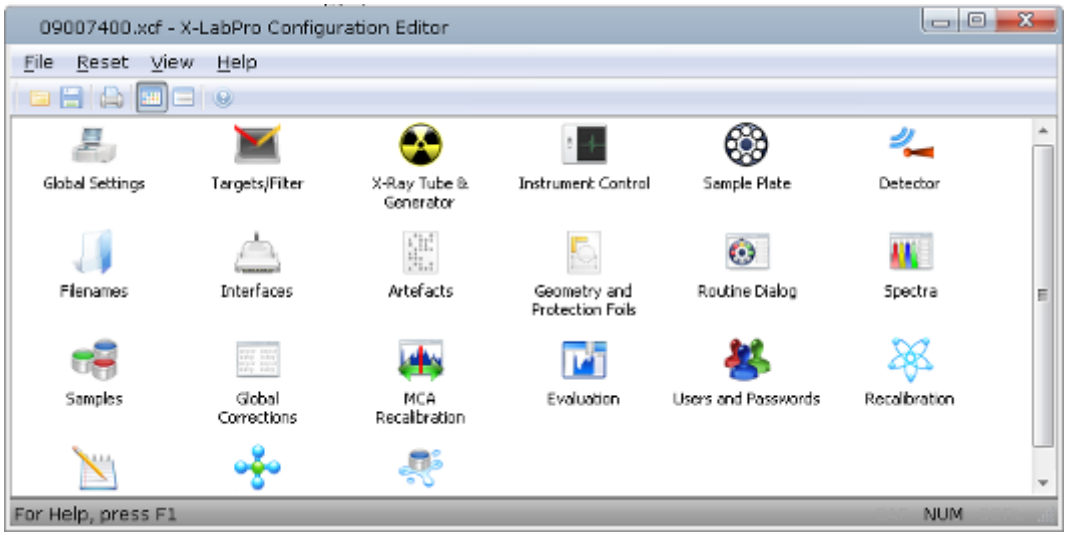
If a sample is deleted, it will not be erased completely. Instead of erasing, the sample is moved into a special job - the Recycle Bin.

If the deleting was made by mistake, the sample can be moved back to its orignal place, where it was stored before deleting.

This only works, if the respective method still exists!

15 Configuration Editor

The *Configuration Editor* can be used to edit a lot of parameters of X-Lab[pro]. Several of them describe SPECTRO inhouse instrument details and therefore they are write-protected.



15.1 User Management

To restrict the access on data and methods by unauthorized persons, it is possible to equip the software with a login procedure.

The user names, user rights and passwords are handled by the User Management, which can be entered in the Configuration Editor by *Users and Passwords*.

Up to 16 users with individual authorization levels are possible. The limitations of the different user levels are listed at the end of this page.

With the *Properties...* button it is possible to change the settings for an existing user.

New users are inserted by using the *Add...* button. Then the *Login Name*, the *Name* (not necessary) and the *Password* can be edited. The password has to be confirmed by retyping under *Retype Password*. Finally the *User Level* has to be assigned.

Non-supervisors have no access to the *User Management*.

The limitations of the different user levels:
A maximum of 16 users can be subordinated with the following user levels:

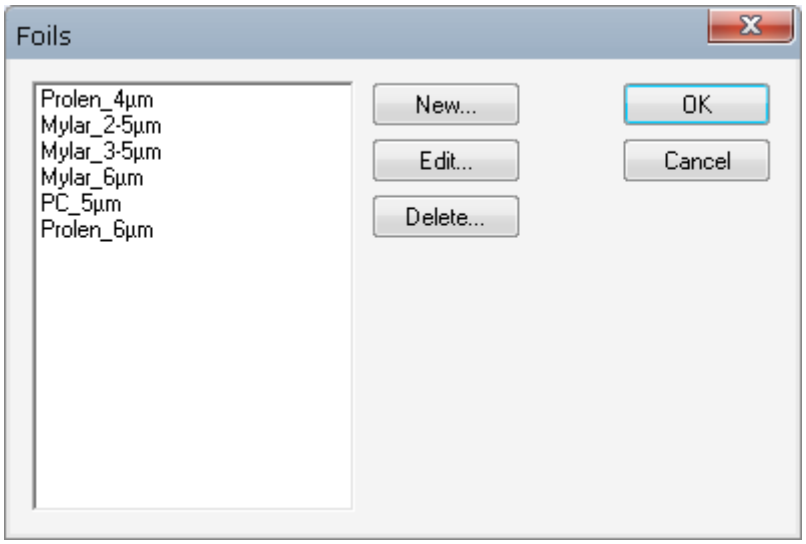
Routine User	The Routine User has only access to the Routine Dialog and not to the main program. This is the lowest user level
Level 3 User	The Level 3 User has only access to the Routine window. He can create new samples, make measurements and analyze samples, but cannot delete them. For this user level a password can be fixed but it isn´t necessary.
Level 2 User	Additionally to the possibilities of the Level 3 user, the Level 2 User also has access to the job and the spectra window. He has the possibility to delete samples and to print results in form of reports.
Level 1 User	The Level 1 user has access to all windows. But in the method window he can only edit non-protected samples or the ones he created himself.

Supervisor	The Supervisor has access to all windows and all options and functions. Only methods delivered from SPECTRO can´t be edited.

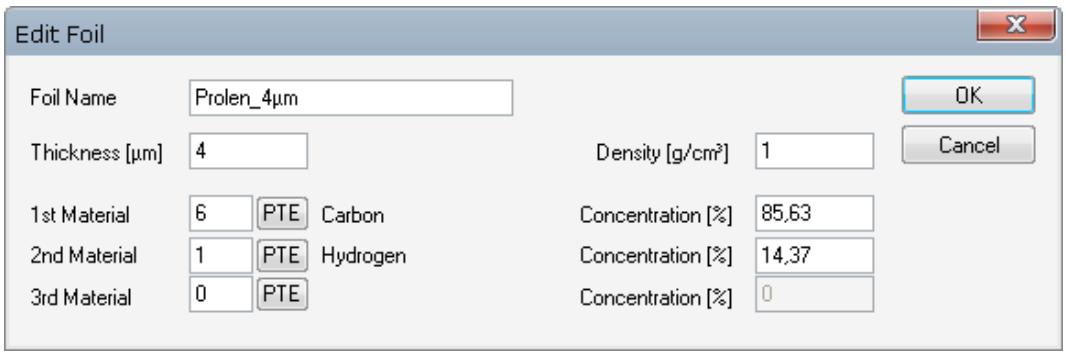
15.2 Definition of Foils

At the general tab in the method window several foils can be selected; the first film for the sample cup (for liquids or powders) and a second film to protect the instrument.

The place to define these foils is the Configuration Editor:



A new type can be added. Existing foils can be deleted or modified:



15.3 Definition of Bonds

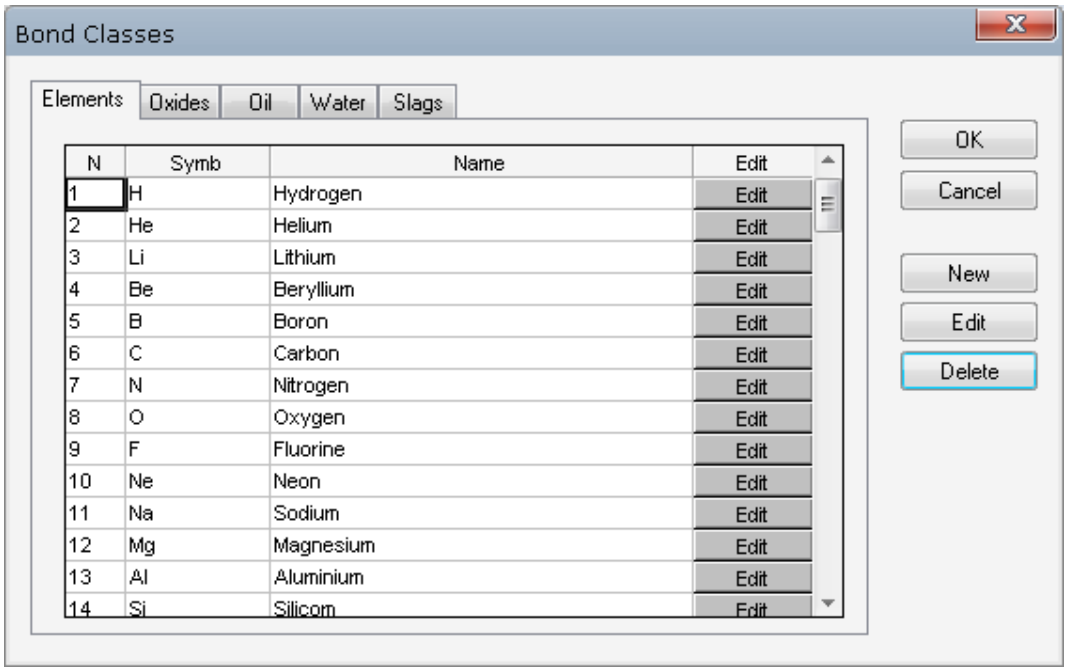
The use of bonds (e.g. as printout option) can be enabled at the method tabs *General* and *Output*.

At the general tab in the method window Bonds can be selected or defined to describe the kind of sample:
If the calculation of concentrations will be done using Fundamental Parameters it can be helpfull/necessary to "tell" the software the chemical state of the elements in the samples: pure elements, oxides, ...
This selection has a big influence on the calculation and its results. Therefore, it is important!

At the Output tab in the method window the option *Bond* is used to define a factor for the presentation of results. Modifications in these bonds will have no influence on the mathematical part: It is only a factor, which is used to calculate the bond, based on the calculatd element concentration.

But, at both tabs (*General* and *Output*) only a pre-defined type of bonds can be selected.
The place to define these bonds and classes of bonds is the Configuration Editor:

The icon *Bonds* gets access to the *Bond Classes*:



New classes can be added, existing types of bonds can be deleted or modified. To modifiy them, use the *Edit* button right to each line:

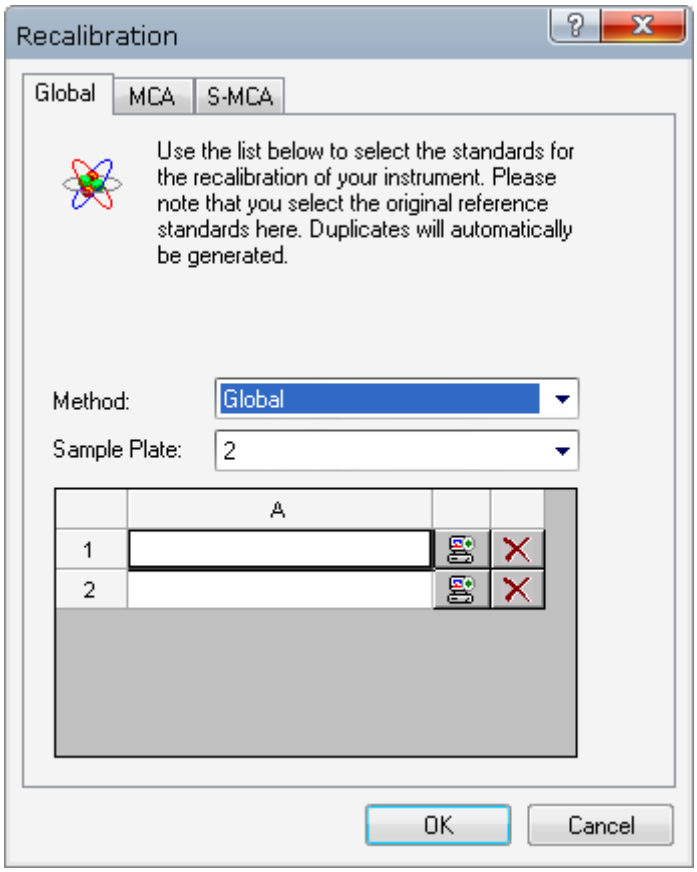
At this screen a new kind of bond can be defined or an existing one can be modified.

To create a new class, decide between starting with an empty class or a copy of an old class.

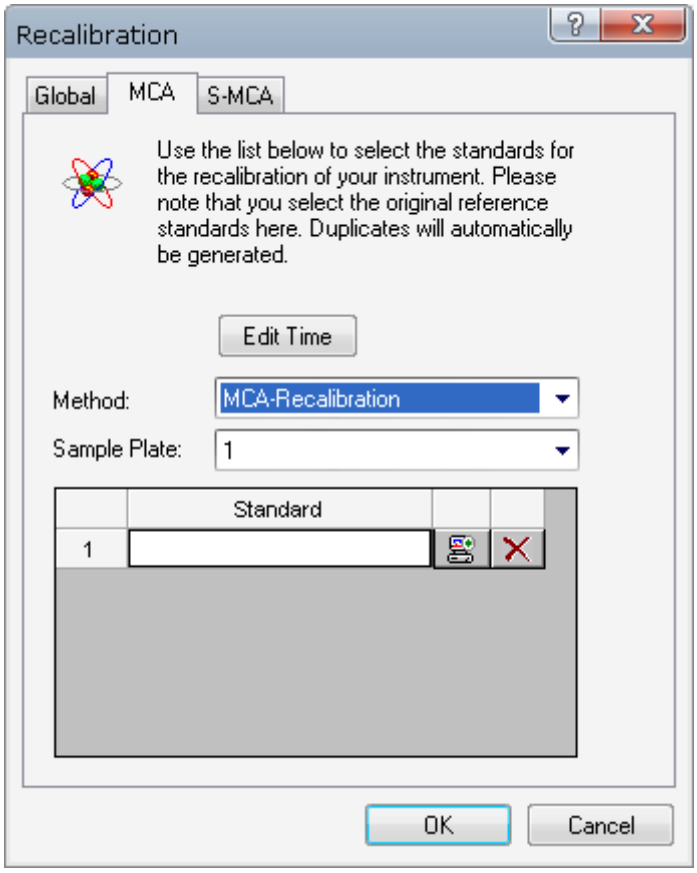
15.4 Definition of Recalibration Samples and Methods

At the General tab in the method window it can be defined, if a method is an analytical one or a special one for recalibration.
If a method is designed as recalibration method it can be used for Global recalibration, Method recalibration, Intercept recalibration or for the Energy-Channel recalibration (MCA).

For each of the named methods/procedures a card exists to define the details:



For both MCA-recalibrations an automatic start of the measurements can be defined.
Therefore, an additional icon *Edit Time* can be found on the card:

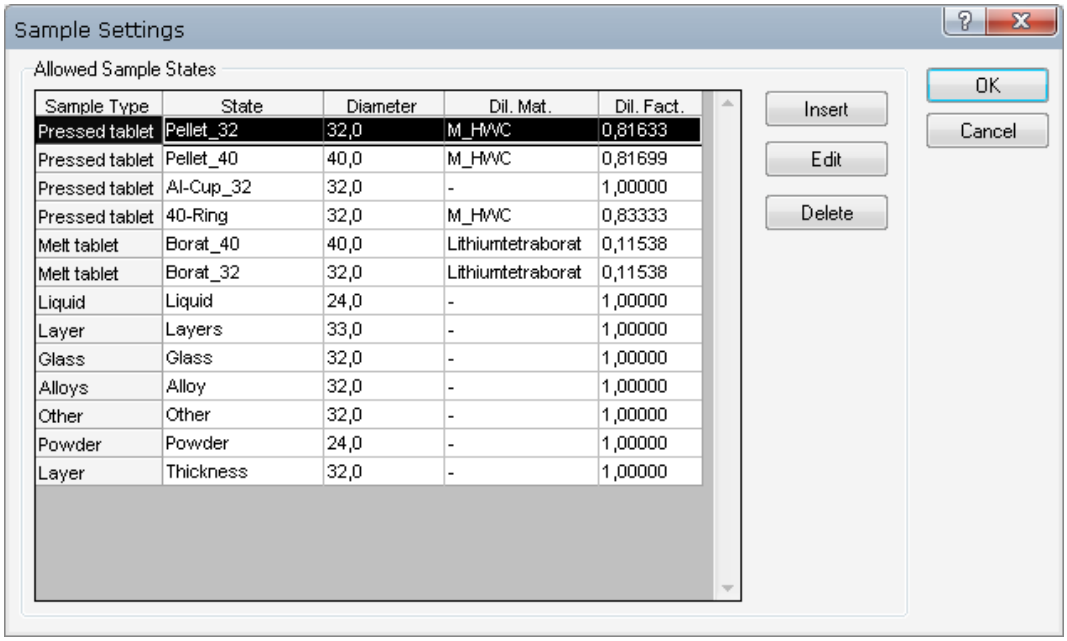


15.5 Definition of Samples

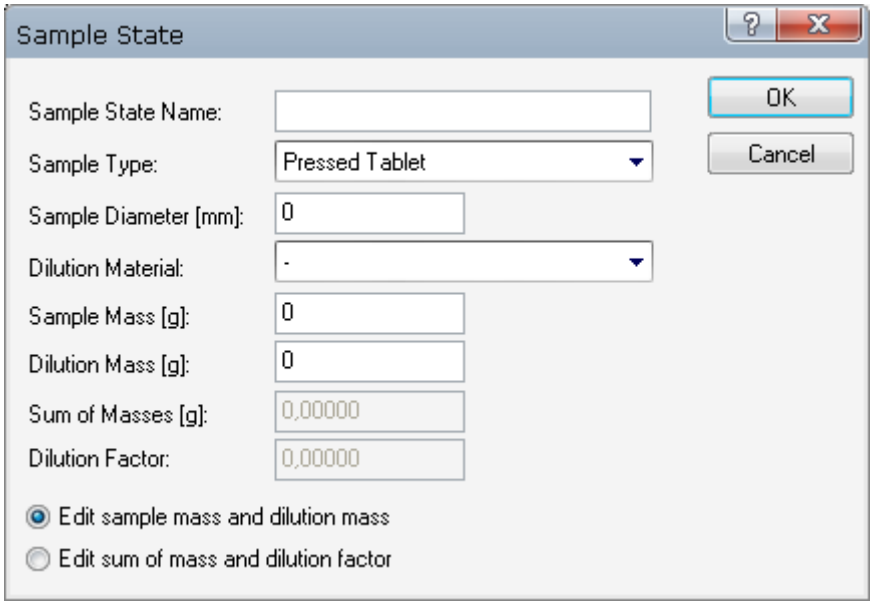
At the General tab in the method window *Sample Type* and *Sample State* are important details to describe a sample. Using the *General* tab, these parameters are defined as the template for all future samples.

In the list of standards the *Sample Type* and *Sample State* can be edited for each sample individually. This can be done, using either the right mouse button and selecting *Edit...* or by selecting *Adopt Defaults* from the *Method* menu.

The available types/states are pre-defined in the Configuration Editor. Click on the icon *Samples* to get access to the following screen:

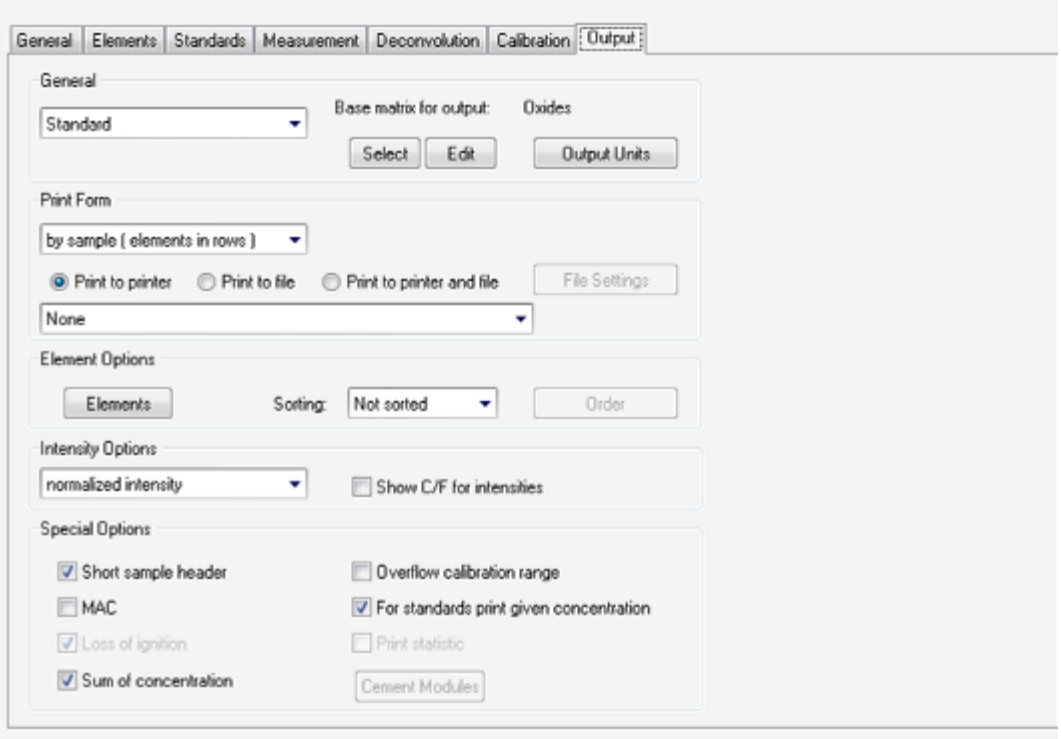

Sample Settings
Allowed Sample States
Sample Type | State | Diameter | Dil. Mat. | Dil. Fact.
Pressed tablet | Pellet_32 | 32,0 | M_HWC | 0,81633
Pressed tablet | Pellet_40 | 40,0 | M_HWC | 0,81699
Pressed tablet | Al-Cup_32 | 32,0 | - | 1,00000
Pressed tablet | 40-Ring | 32,0 | M_HWC | 0,83333
Melt tablet | Borat_40 | 40,0 | Lithiumtetraborat | 0,11538
Melt tablet | Borat_32 | 32,0 | Lithiumtetraborat | 0,11538
Liquid | Liquid | 24,0 | - | 1,00000
Layer | Layers | 33,0 | - | 1,00000
Glass | Glass | 32,0 | - | 1,00000
Alloys | Alloy | 32,0 | - | 1,00000
Other | Other | 32,0 | - | 1,00000
Powder | Powder | 24,0 | - | 1,00000
Layer | Thickness | 32,0 | - | 1,00000
Insert
Edit
Delete
OK
Cancel

A new Sample State/Sample Type can be *inserted* or *edited*/*deleted* (see below):



16 General

This tab is the main tab in the method window. It allows to edit the most important parameters of a method:



The parameters in this screen are:

Global Settings:
In this section some global settings can be defined, like name of the method or sample state.
One of the most important parameters is called *Mathematics*. It describes the mathematical procedure used for calibration and evaluation.
The parameter *Option* is used to define, whether a method will be used as an analytical method (Standard) or for recalibrations (e.g. MCA).

Dilution:
It describes the default settings for a new sample, which will be created during routine use of this method.
The dilution material and the masses defined here will be used later.

Additional Settings:
This section contains the diameter of the sample, information about foils and the standard for comparison.

Normalization:
Here, the different possible normalization options can be selected:
- Normalize results: The results will be normalized e.g. to 100%.
- MSK: The *Mass Attenuation Coefficient* is used to calculate the "non-visible part" (elements with atomic number < 10) of the sample.

Accordingly, the results can be normalized to the "visible part".
- Difference element: This can be used to tell the mathematical procedure, what's the "non-visible" part of the sample.This can be e.g. CH2 for an oil sample, H2O for a water sample or Oxygen for a slag...

16.1 Recalibration

An existing calibration is based on the relation between a known concentration and a measured count rate. Whenever this count rate is changing with time, it is necessary to either calibrate the instrument again or to recalibrate it. The number of standards to run a recalibration is much less than for an initial calibration.

A recalibration is necessary, if the count rates change or if the excitation geometry of the instrument was modified. During a recalibration the ratio of the original count rates (at the moment of the calibration) to the actual count rates are calculated. This ratio is used as a correction factor for the original calibration.

Recently measured count rates are multiplied by the correction factor and then the old calibration curves can be used. The X-Lab^{Pro} software supports three different kinds of correction factors:

- target correction factors
- global correction factors
- method correction factors

If the correction factor for all elements, analyzed with a specific target, is the same, a target correction factor is used. If the difference between the correction factors is too large, an individual global correction factor for each element has to be used. Global and target correction factors affect all methods, so if only a specific method should be recalibrated, method correction factors must be used.

A recalibration is automatically in use from the instant of running it. With the exception of target correction factors, the correction factors are even used, when old measurements are reevaluated.

Two different recalibration procedures exist.

- Global recalibration
- Method recalibration

The *global recalibration* can be used to correct influences that are affecting all methods in the same way. This includes a drift correction due to aging of components (e.g. x-ray tube, detection system) or changes in the geometry or excitation conditions (e.g. changed protection film material).

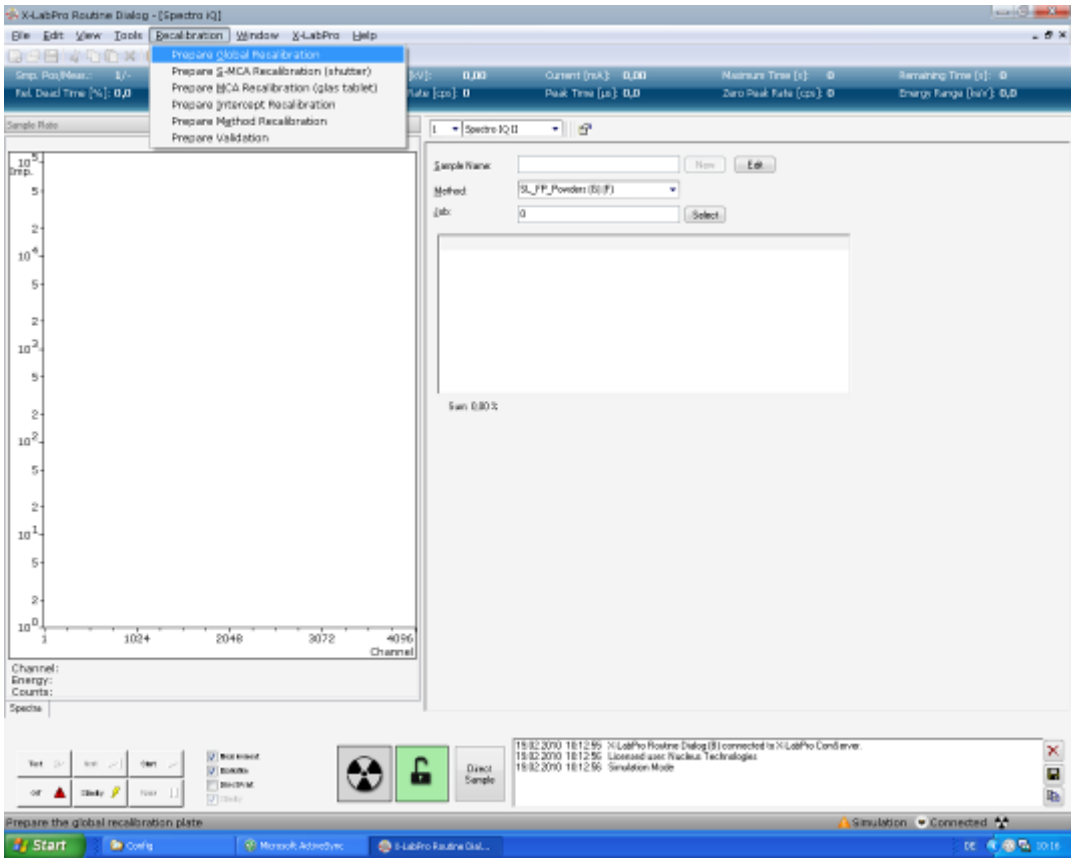
The *method recalibration* is only affecting the selected method and therefore has a completely different application. The method recalibration should be used when the modification of the geometry is only affecting a specific method. This can be a modified purge gas (nitrogen instead of helium) or a different foil for the preparation of cuvettes.

For both types of recalibration the software offers special routines to simplify these procedures. They can be adjusted in the Configuration Editor.

16.2 Global Recalibration

To correct for global effects that are affecting all methods in the same way the global recalibration must be used. The easiest way to do this is to use a special set of glass beads. The method containing the glass samples is typically called *Global*.

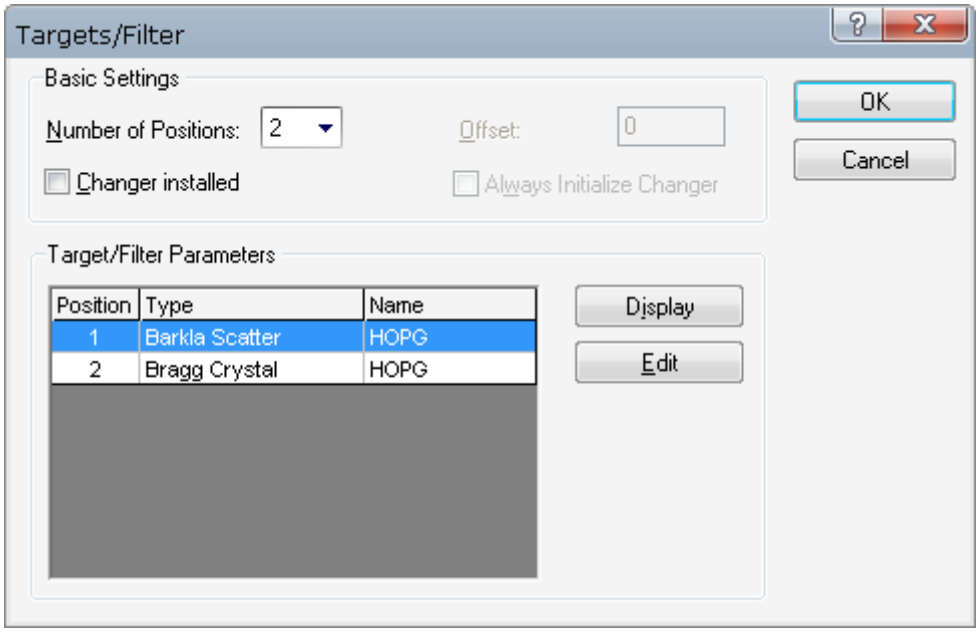
To do the Global Recalibration select *Prepare Global Recalibration* from the menu *Recalibration*.



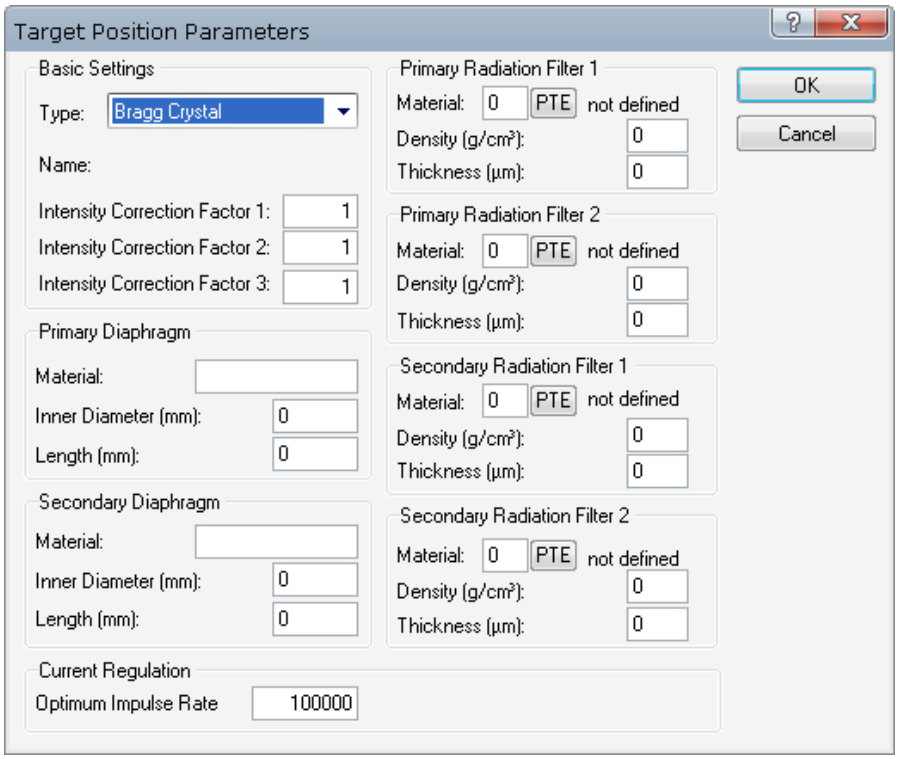
The recalibration procedure starts by selecting the *Start* button.

After the measurements and evaluations are finished, the software automatically calculates the correction factors.
These are written in the instrument configuration file. Additionally, the results of the recalibration are stored in a text file named "GlobalRecalibration.txt" in the directory C:\Xlabpro\LogFiles.

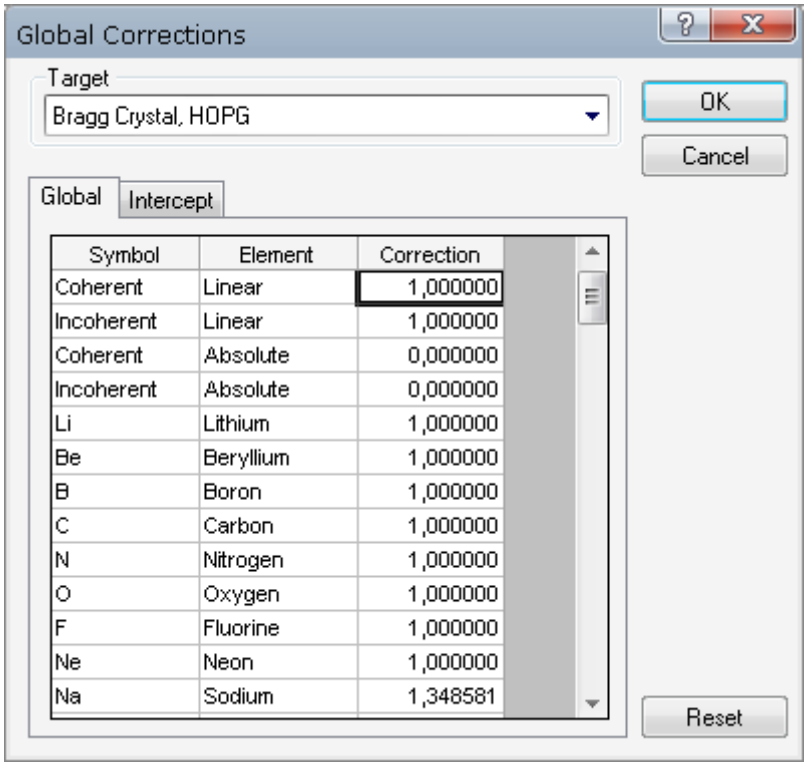
The calculated correction may be the target correction factors or element specific global correction factors.
Both are stored in the configuration file of the instrument, but at different places.
Target correction factors can be found in the **configuration editor** under *Targets/Filter*,
while the **global correction** factors are strored under *Global Corrections*.



To view the **target correction** factors, the appropriate target has to be selected and then the *Display* button has to be used.
An alternative way is to double click on the desired target.
The target correction factor is named *Intensity Correction Factor*.



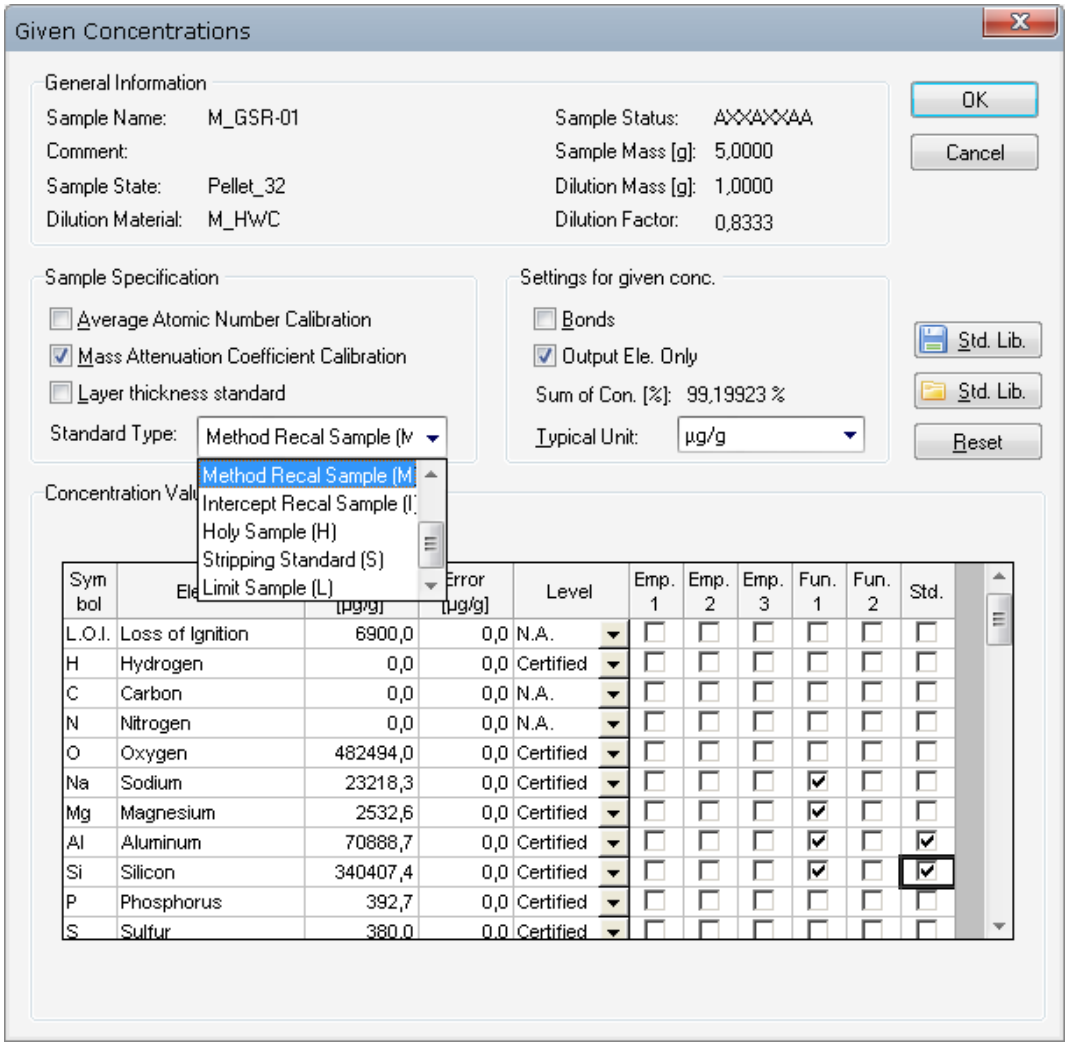
The **global correction** factors can be shown for each of the installed targets of an instrument by selecting "Global corrections" in the **configuration editor**. After selecting a target, the correction factors are shown in the table.



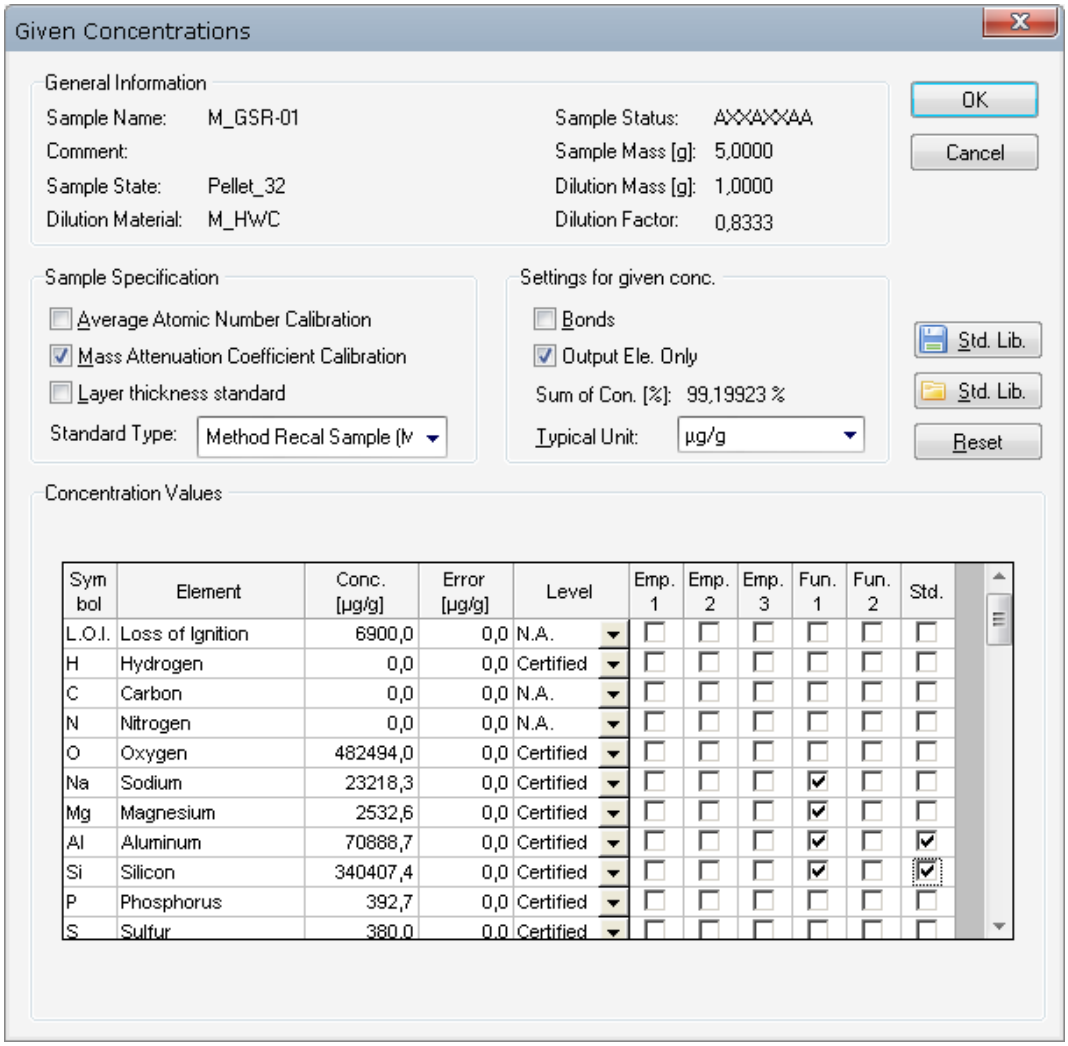
16.3 Method Recalibration

In comparison to the global recalibration, that is used to correct influences affecting all methods in a similar way,
the Method Recalibration is used to adjust a specific method without affecting the other methods.
This can be necessary, when the measurement conditions of a method have been changed (e.g. if a different purge gas or protection foil are used).

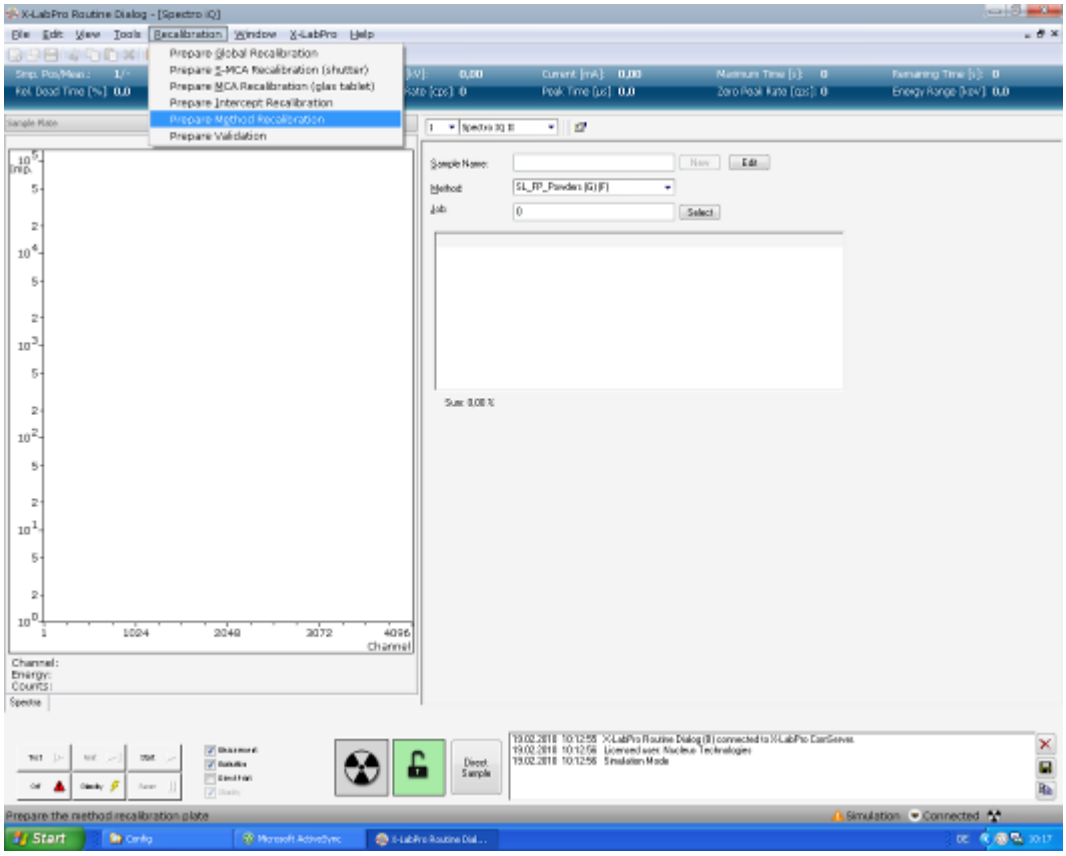
To do the Method Recalibration select minimum one sample from the method as recalibration sample.

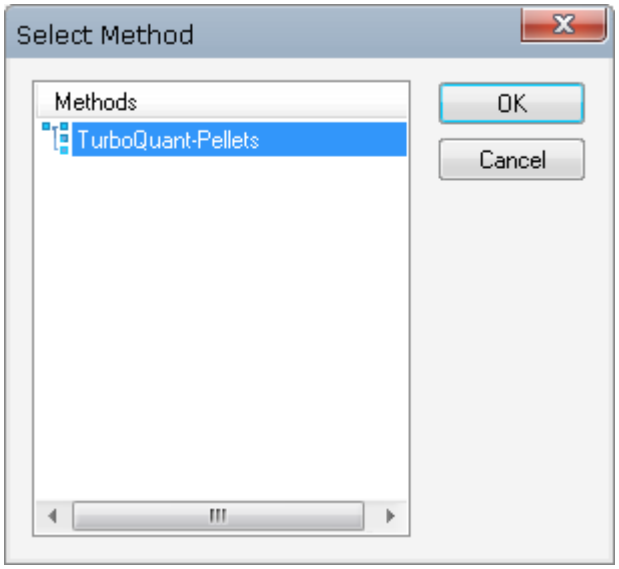


Define the elements, which you want to use from this sample by marking the tick box for Std. at the given concentrations of this sample.


Given Concentrations
General Information
Sample Name: M_GSR-01
Comment:
Sample State: Pellet_32
Dilution Material: M_HWC
Sample Status: AXXAXXAA
Sample Mass [g]: 5,0000
Dilution Mass [g]: 1,0000
Dilution Factor: 0,8333
OK
Cancel
Sample Specification
Average Atomic Number Calibration
Mass Attenuation Coefficient Calibration
Layer thickness standard
Standard Type: Method Recal Sample (M
Settings for given conc.
Bonds
Output Ele. Only
Sum of Con. [%]: 99,19923 %
Typical Unit: µg/g
Std. Lib.
Std. Lib.
Reset
Concentration Values
Symbol | Element | Conc. [µg/g] | Error [µg/g] | Level | Emp. 1 | Emp. 2 | Emp. 3 | Fun. 1 | Fun. 2 | Std.
L.O.I. | Loss of Ignition | 6900,0 | 0,0 | N.A.
H | Hydrogen | 0,0 | 0,0 | Certified
C | Carbon | 0,0 | 0,0 | N.A.
N | Nitrogen | 0,0 | 0,0 | N.A.
O | Oxygen | 482494,0 | 0,0 | Certified
Na | Sodium | 23218,3 | 0,0 | Certified
Mg | Magnesium | 2532,6 | 0,0 | Certified
Al | Aluminum | 70888,7 | 0,0 | Certified
Si | Silicon | 340407,4 | 0,0 | Certified
P | Phosphorus | 392,7 | 0,0 | Certified
S | Sulfur | 380,0 | 0,0 | Certified

In the routine dialog select the *Prepare Method Recalibration* from the menu *Recalibration*.

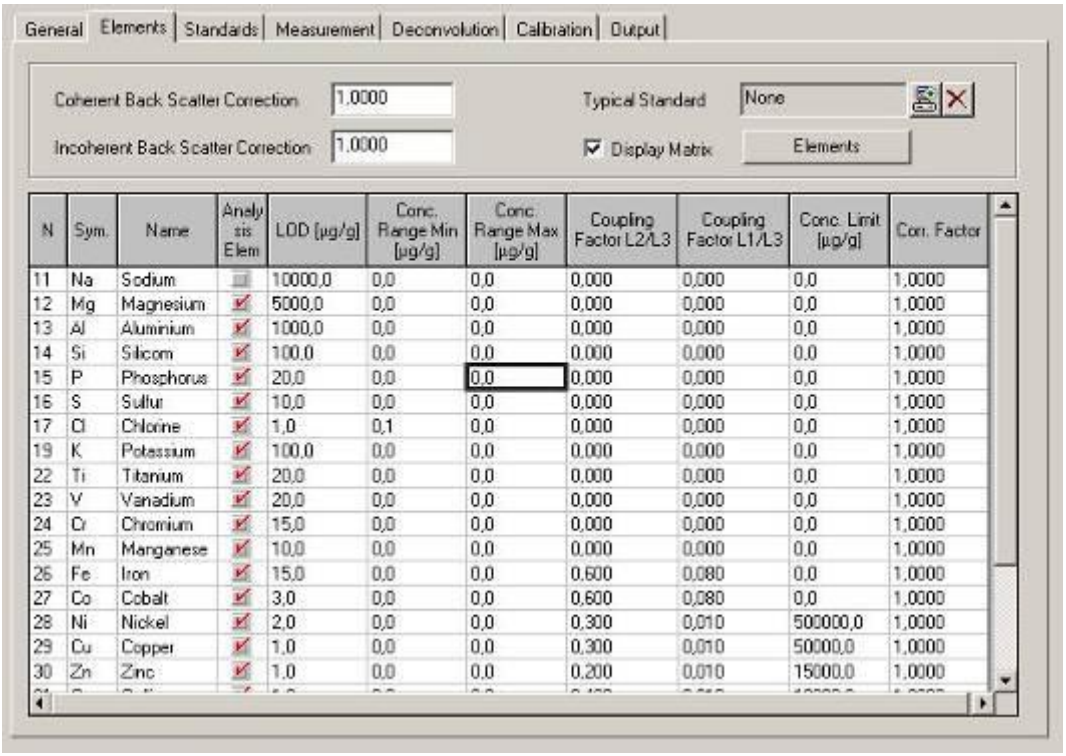




The recalibration procedure is started by selecting the *Start* button.

After the measurements and evaluations are finished, the software automatically calculates correction factors. Additionally, the results of the recalibration are stored in a text file named "MethodRecalibration.txt" in the directory C:\Xlabpro\LogFiles. Please note that the according method needs to be closed during evaluation progress!

The correction factors are automatically stored in the method. To check or adjust them manually, the Method Administration must be selected in the sub-module Elements. In the last column one can find the correction factors (*Corr.factor*).

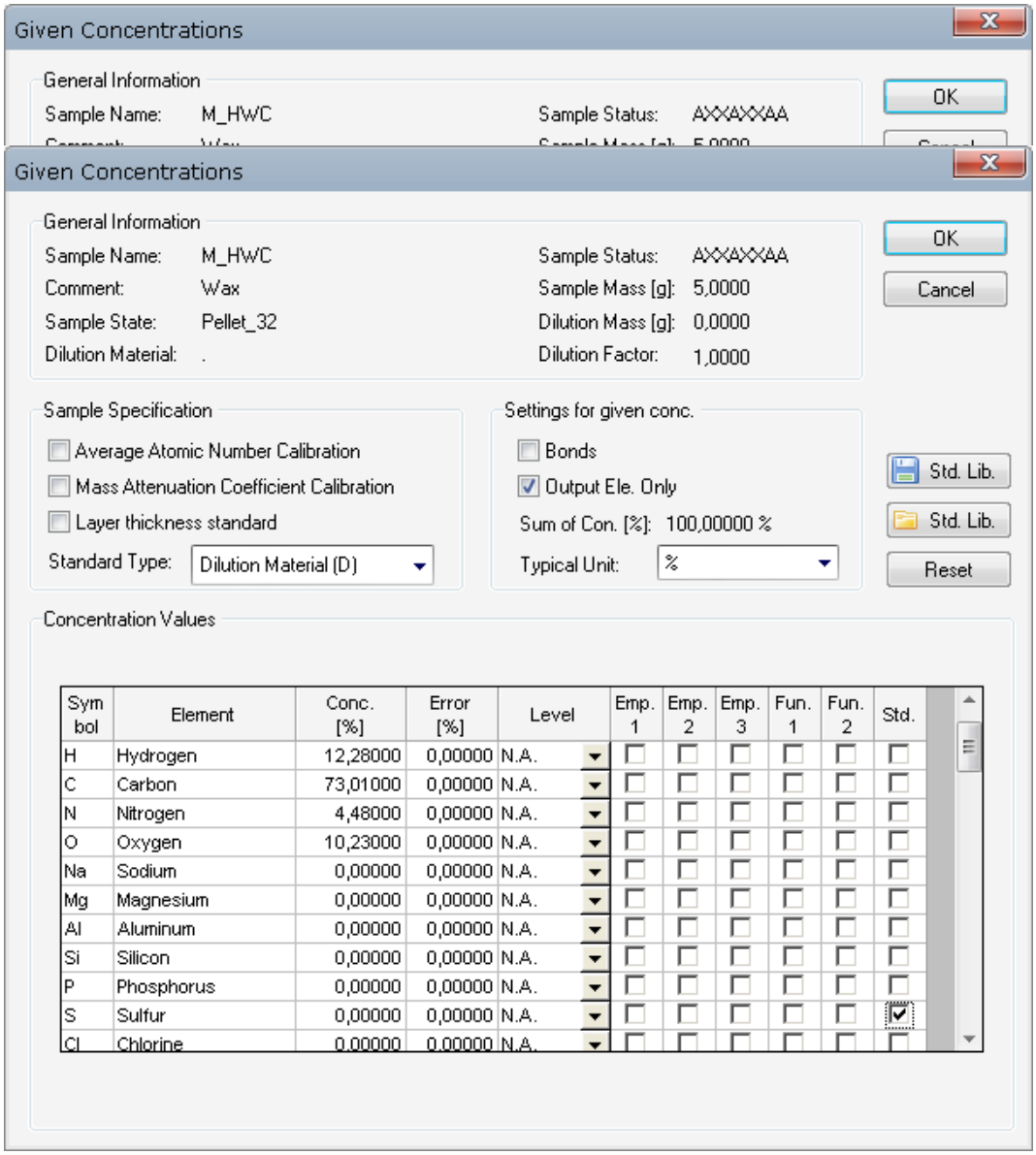


N	Sym.	Name	Analysis Elem	LOD [µg/g]	Conc. Range Min [µg/g]	Conc. Range Max [µg/g]	Coupling Factor L2/L3	Coupling Factor L1/L3	Conc. Limit [µg/g]	Corr. Factor
11	Na	Sodium		10000,0	0,0	0,0	0,000	0,000	0,0	1,0000
12	Mg	Magnesium	✓	5000,0	0,0	0,0	0,000	0,000	0,0	1,0000
13	Al	Aluminium	✓	1000,0	0,0	0,0	0,000	0,000	0,0	1,0000
14	Si	Silicom	✓	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
15	P	Phosphorus	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
16	S	Sulfur	✓	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
17	Cl	Chlorine	✓	1,0	0,1	0,0	0,000	0,000	0,0	1,0000
19	K	Potassium	✓	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
22	Ti	Titanium	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
23	V	Vanadium	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
24	Cr	Chromium	✓	15,0	0,0	0,0	0,000	0,000	0,0	1,0000
25	Mn	Manganese	✓	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
26	Fe	Iron	✓	15,0	0,0	0,0	0,600	0,080	0,0	1,0000
27	Co	Cobalt	✓	3,0	0,0	0,0	0,600	0,080	0,0	1,0000
28	Ni	Nickel	✓	2,0	0,0	0,0	0,300	0,010	500000,0	1,0000
29	Cu	Copper	✓	1,0	0,0	0,0	0,300	0,010	50000,0	1,0000
30	Zn	Zinc	✓	1,0	0,0	0,0	0,200	0,010	15000,0	1,0000

16.4 Intercept Recalibration

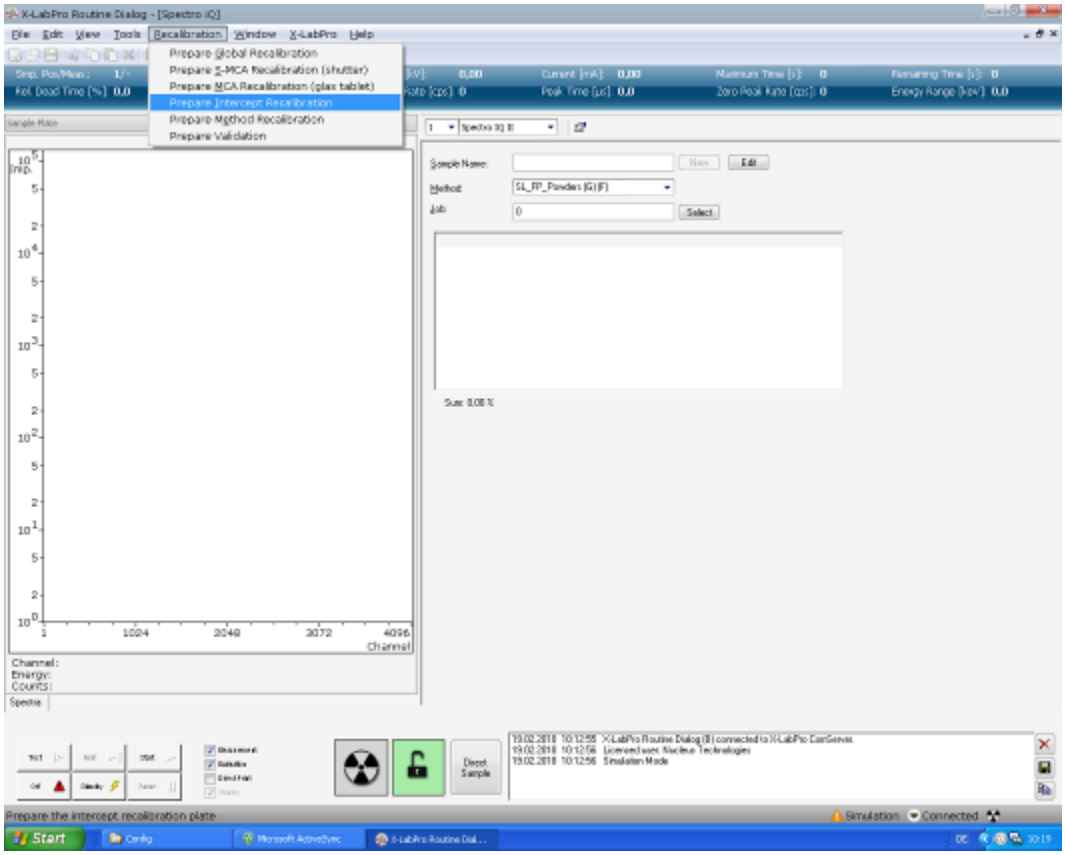
A special kind of recalibration can be used, if analysis very close to detection limit will be done.
This Intercept Recalibration is especially created for the Low-Sulfur-Application. Running this, recalibration the offset of the Sulfur calibration will be recalculated to adjust the instrument after a long time of using.

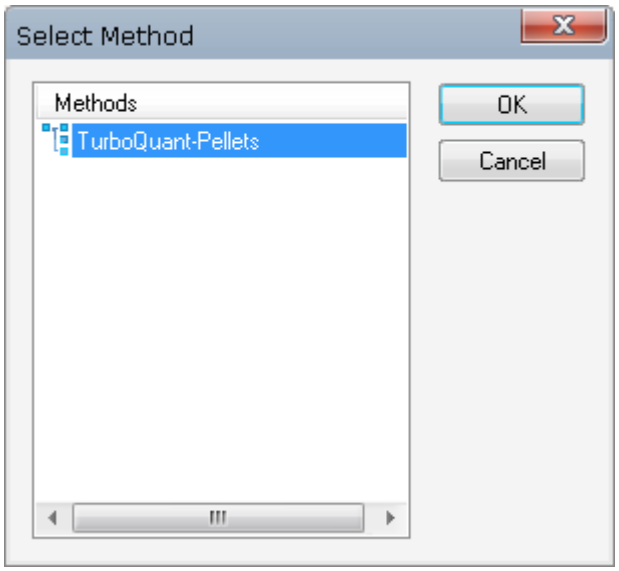
To do the Intercept Recalibration select minimum one sample from the method as recalibration sample.



To do the Intercept Recalibration the recalibration sample(s) have to be in the defined positions of the sample plate.
Select the *Prepare Intercept Recalibration* from the menu *Recalibration*.

Please note that the respective method needs to be closed during evaluation progress!

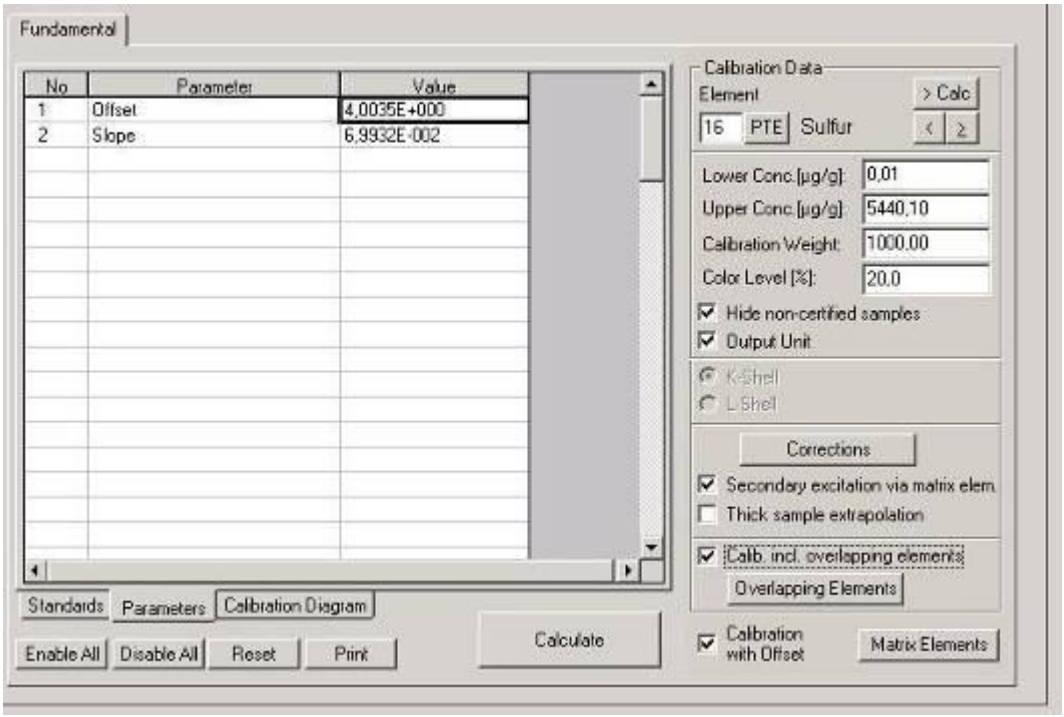




The recalibration procedure is started by selecting the *Start* button.

After the measurements and evaluations are finished, the software calculates automatically the new offset.

The offset is automatically stored in the method. To check or adjust it manually the method must be selected in the sub-module *Calibration* of the *Method Administration* module.
After selecting the tab *Parameters* the offset is displayed as the first parameter, called "Offset" (in this example 4.0035).

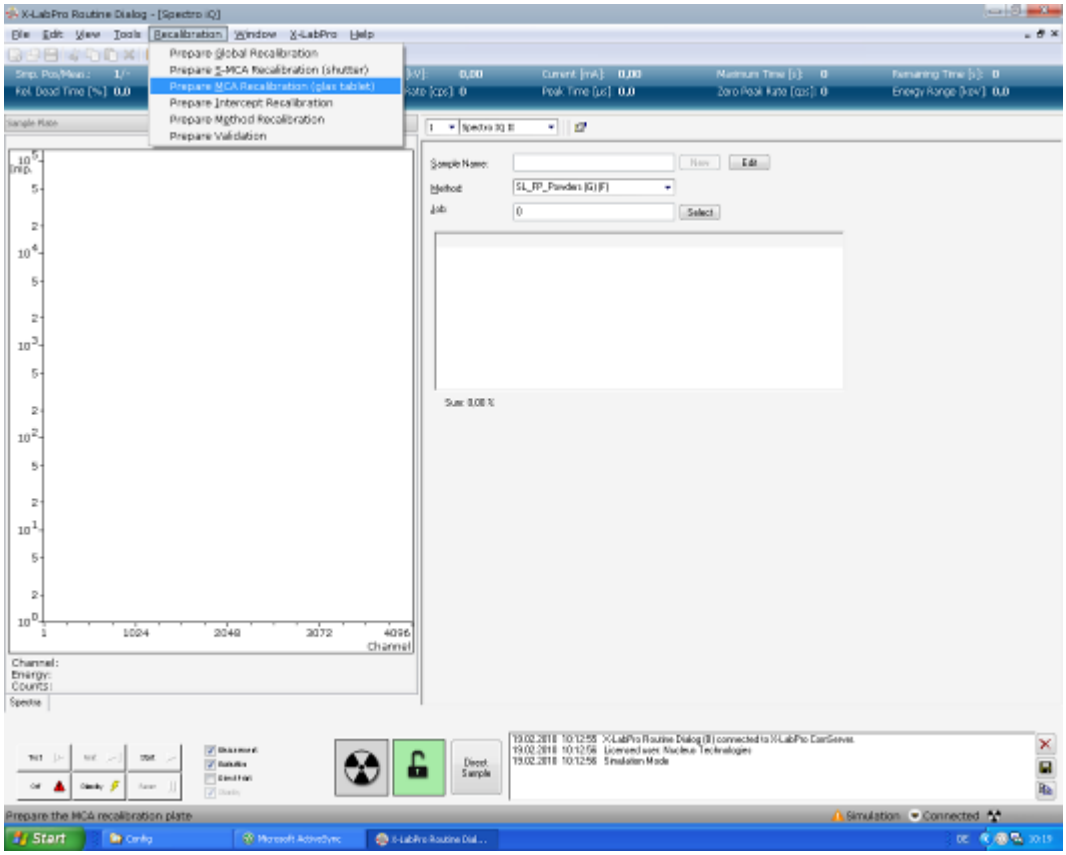


16.5 Run MCA Calibration

The energy channel calibration, also known as MCA (Multi Channel Analyzer) calibration should be performed once a week.

The first MCA calibration is done in Kleve measuring a glass bead and calculating several parameters.

To check this calibration (once a week), this glass bead has to be measured again.
To do this, select the *Prepare MCA Calibration (glas tablet)* from the menu *Recalibration:*
A sample with a new extension is created, automatically.



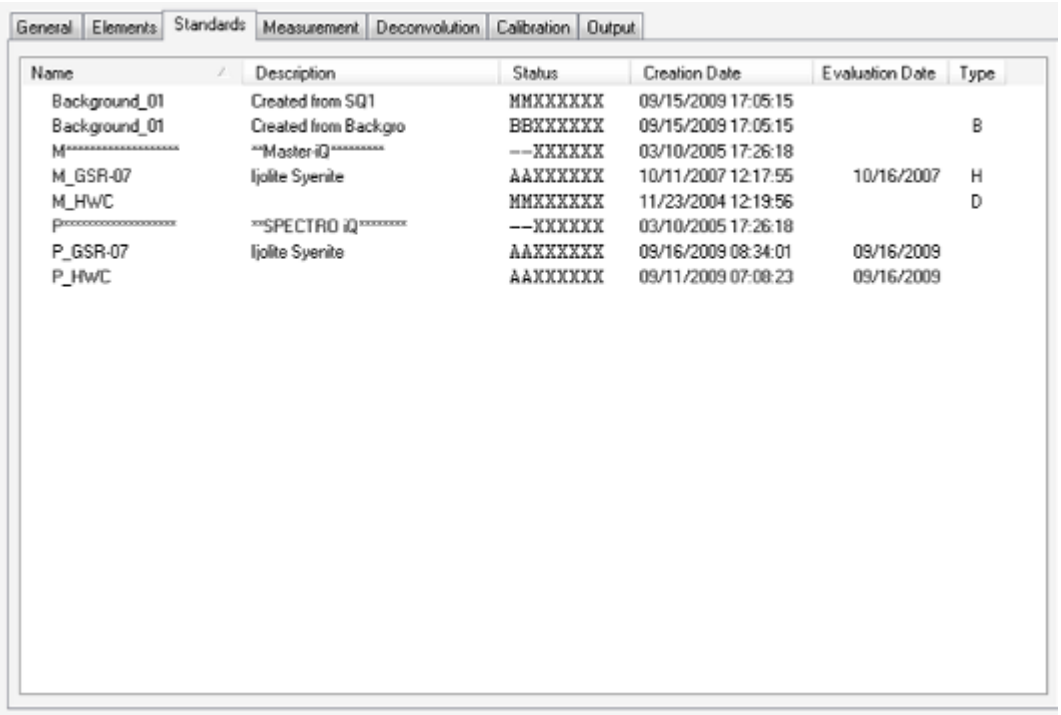
To start the MCA calibration, select the *Start* button (with enabled *Evaluation* box right hand of the *Start* button).

To configure it, use the Configuration Editor.

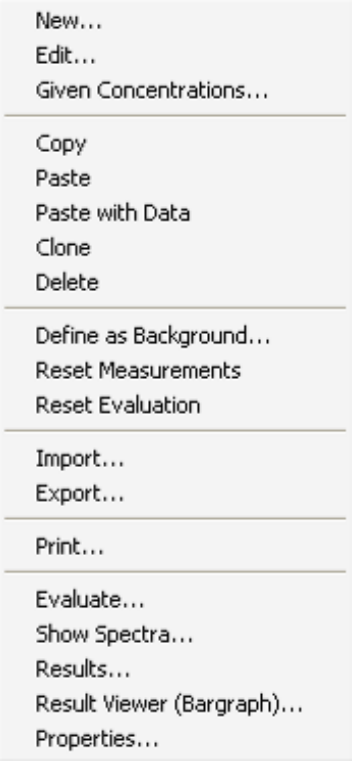
This MCA can also be used in combination with a Global Recalibration.

16.6 Standards

The method comprises the calibration standards. These can be edited at the tab *Standards*.



It contains different columns which can be used to change the order of presentation.

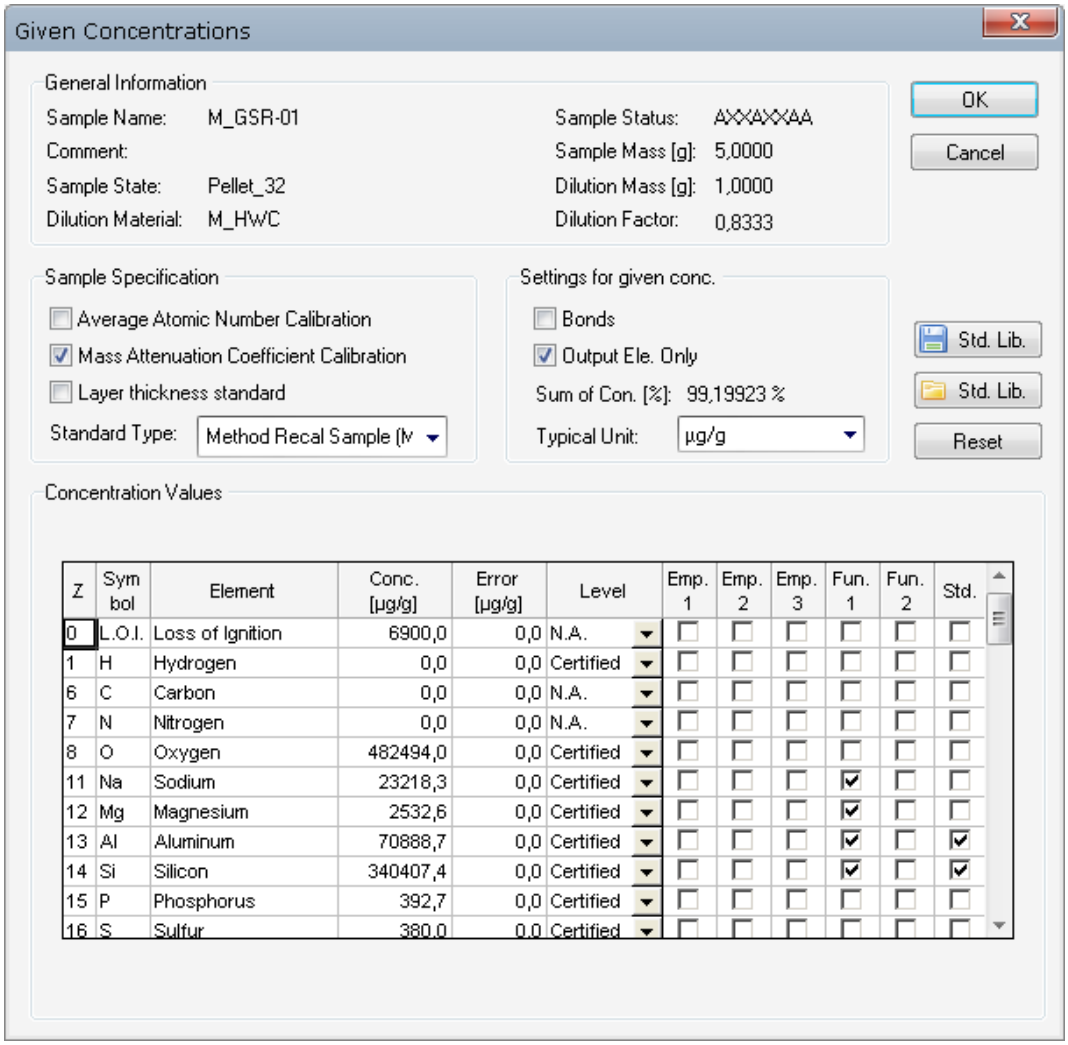


Using the right mouse button a context menu gives access to all important functions regarding standard samples.

One of them is the given concentrations, which are necessary for calibration.
Especially for the non-empirical procedures like Fundamental Parameter Models or Spectro procedure, it is important to tell the software all available informations, because these mathematical procedures require a 100%-knowledge.
E.g. we cannot determine Oxygen. But, if you know, that elements in a sample are bonded as oxides, you should edit the Oxygen concentration - independent from the fact, that it will not be calibrated.

In addition some shortcuts are introduced like "Show Spectra...". Without using the clipboard the selected sample will be copied into the Spectra Viewer.

Given Concentrations:


Given Concentrations
General Information
Sample Name: M_GSR-01
Comment:
Sample State: Pellet_32
Dilution Material: M_HWC
Sample Status: AXXAXXAA
Sample Mass [g]: 5,0000
Dilution Mass [g]: 1,0000
Dilution Factor: 0,8333
OK
Cancel
Sample Specification
Average Atomic Number Calibration
Mass Attenuation Coefficient Calibration
Layer thickness standard
Standard Type: Method Recal Sample (M
Settings for given conc.
Bonds
Output Ele. Only
Sum of Con. [%]: 99,19923 %
Typical Unit: µg/g
Std. Lib.
Std. Lib.
Reset
Concentration Values
Z | Symbol | Element | Conc. [µg/g] | Error [µg/g] | Level | Emp. 1 | Emp. 2 | Emp. 3 | Fun. 1 | Fun. 2 | Std.
0 | L.O.I. | Loss of Ignition | 6900,0 | 0,0 | N.A.
1 | H | Hydrogen | 0,0 | 0,0 | Certified
6 | C | Carbon | 0,0 | 0,0 | N.A.
7 | N | Nitrogen | 0,0 | 0,0 | N.A.
8 | O | Oxygen | 482494,0 | 0,0 | Certified
11 | Na | Sodium | 23218,3 | 0,0 | Certified
12 | Mg | Magnesium | 2532,6 | 0,0 | Certified
13 | Al | Aluminum | 70888,7 | 0,0 | Certified
14 | Si | Silicon | 340407,4 | 0,0 | Certified
15 | P | Phosphorus | 392,7 | 0,0 | Certified
16 | S | Sulfur | 380,0 | 0,0 | Certified

This window is to define the given concentrations - the goal of the calibration.
As mentioned before, it can be necessary for FPM to describe the sample 100 % (if all these concentrations are of interest or not!).

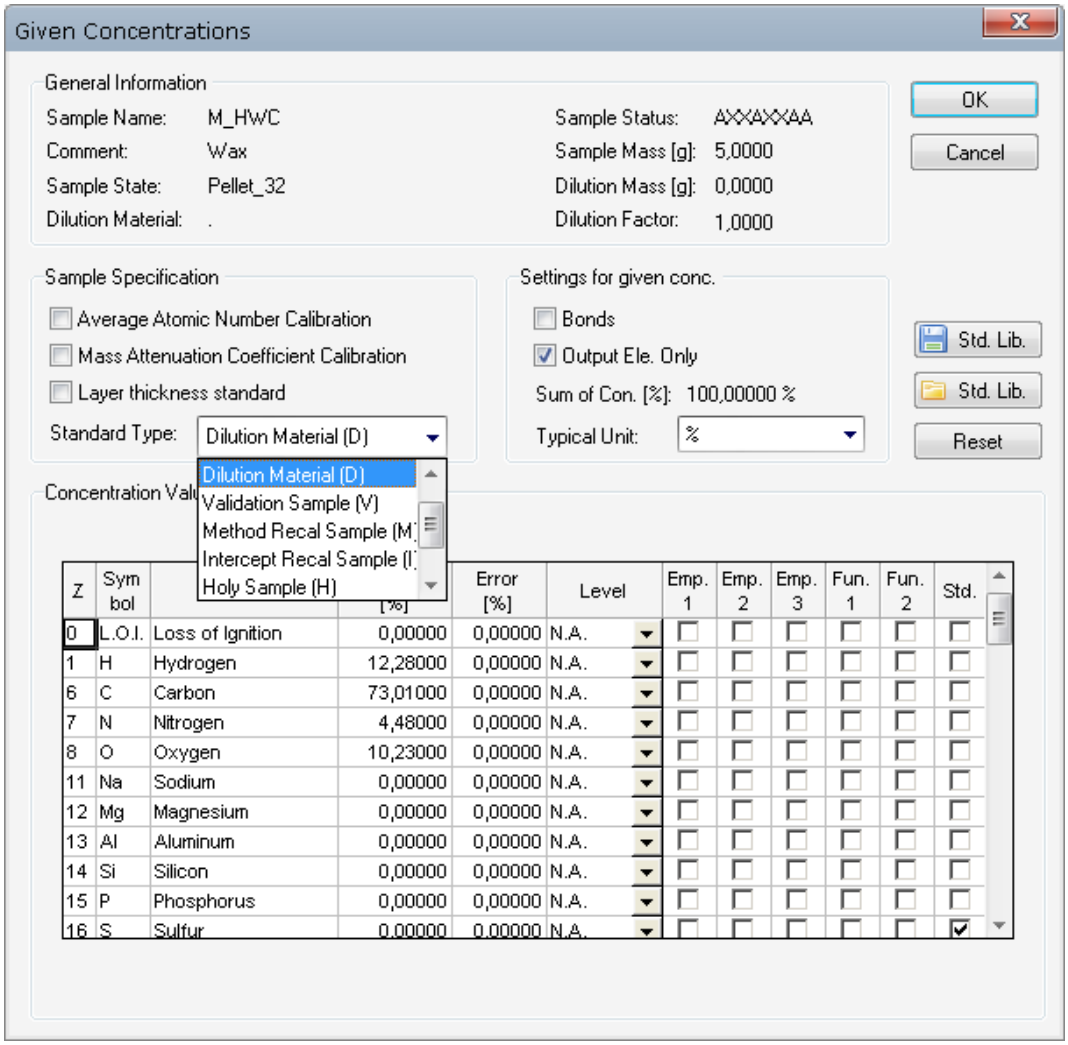
The first details, which should fit to the sample and its given concentrations should be the ***Typical Unit***.
This should be the right one before entering concentrations. It can be changed at each time, but BEFORE entering a number. Changes of the unit afterwards will have no influence to "old" concentrations.

To make it more comfortable, if bonds like Oxides are to define, the feature "***Bonds***" can be used. A sum is counting all defined concentrations as additional control option.

In the list in the lower part of this screen all elements ALL elements - (independent from selections) are visible. A concentration, the error of this concentration and the level of cerification can be defined.

The last 5 columns are not really important, because there's another location to get access to the informations stored here.

Dilution Material:
If the sample should be a new Dilution material, that can be selected for new routine samples, this should be selected.


Given Concentrations
General Information
Sample Name: M_HWC
Comment: Wax
Sample State: Pellet_32
Dilution Material: .
Sample Status: AXXAXXAA
Sample Mass [g]: 5,0000
Dilution Mass [g]: 0,0000
Dilution Factor: 1,0000
OK
Cancel
Sample Specification
Average Atomic Number Calibration
Mass Attenuation Coefficient Calibration
Layer thickness standard
Standard Type: Dilution Material (D)
Dilution Material (D)
Validation Sample (V)
Method Recal Sample (M)
Intercept Recal Sample (I)
Holy Sample (H)
Settings for given conc.
Bonds
Output Ele. Only
Sum of Con. [%]: 100,00000 %
Typical Unit: %
Std. Lib.
Std. Lib.
Reset
Concentration Valu
Z | Symbol | [%] | Error [%] | Level | Emp. 1 | Emp. 2 | Emp. 3 | Fun. 1 | Fun. 2 | Std.
0 L.O.I. Loss of Ignition 0,00000 0,00000 N.A.
1 H Hydrogen 12,28000 0,00000 N.A.
6 C Carbon 73,01000 0,00000 N.A.
7 N Nitrogen 4,48000 0,00000 N.A.
8 O Oxygen 10,23000 0,00000 N.A.
11 Na Sodium 0,00000 0,00000 N.A.
12 Mg Magnesium 0,00000 0,00000 N.A.
13 Al Aluminum 0,00000 0,00000 N.A.
14 Si Silicon 0,00000 0,00000 N.A.
15 P Phosphorus 0,00000 0,00000 N.A.
16 S Sulfur 0,00000 0,00000 N.A.

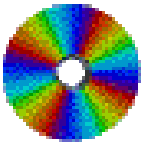
Std-. Lib.:
The Standard-Library (or Library of Standards) is a tool to accelerate the definition of the given concentrations, if a well-known, certified standard is used:
Many of these Certified Reference Materials (CRM) are pre-defined in the Library of Standards and own standards can be added.
To use the stored data or to add the actual sample into this library, these buttons can be used.

17 Data Storage

The User of the Spectro X-Lab[Pro] software is fully responsible for data storage and backup copies!!!

We - as SPECTRO - have prepared a backup of your instrument specific data before shipment of the instrument, but we are not able to store / to archive the data you have measured after delivery / installation.

Therefore, it is your responsibility to assure a regular data storage.
We suggest to copy the complete c:\xlabpro directory to a CD.
If you need to restore your data, please do not hesitate to contact us for details on how to restore.



In addition to such a complete backup, there are different storage options:

The software offers tools to export measurements, methods or jobs from the database structure to allow data storage and data transmission.

The motivation to store methods, jobs and samples is quite different:

· Methods do not change very often so the main motivation is to get some backup copies.
· If a new method will not work properly and will need some assistance from us, the method can be transmitted to us.
· A new method was developed on another computer. After finishing the calibration, it can be copied to the instrument computer.

Export Methods Import Methods

· Jobs contain the routine measurements and here the archiving is the main reason.

Export Jobs Import Jobs

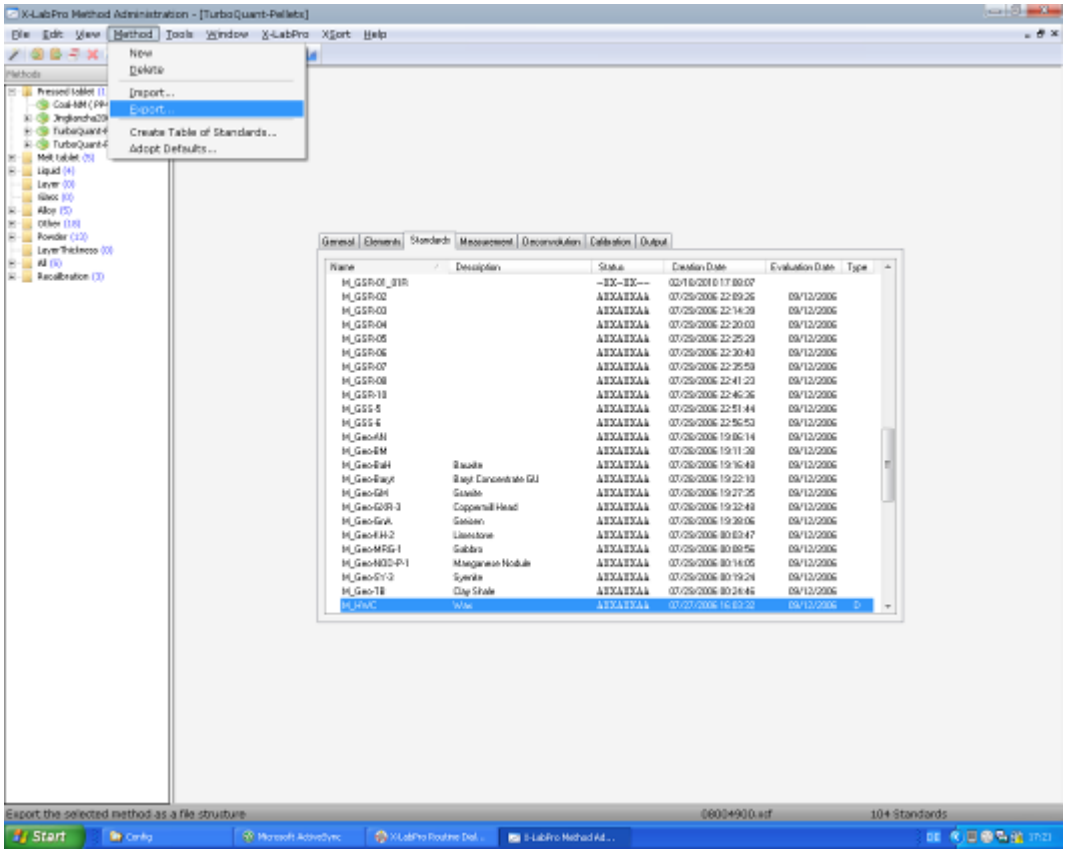
· Single samples are exported to make them available to other users (e.g. SPECTRO).

Export Samples Import Samples

18 Import/Export

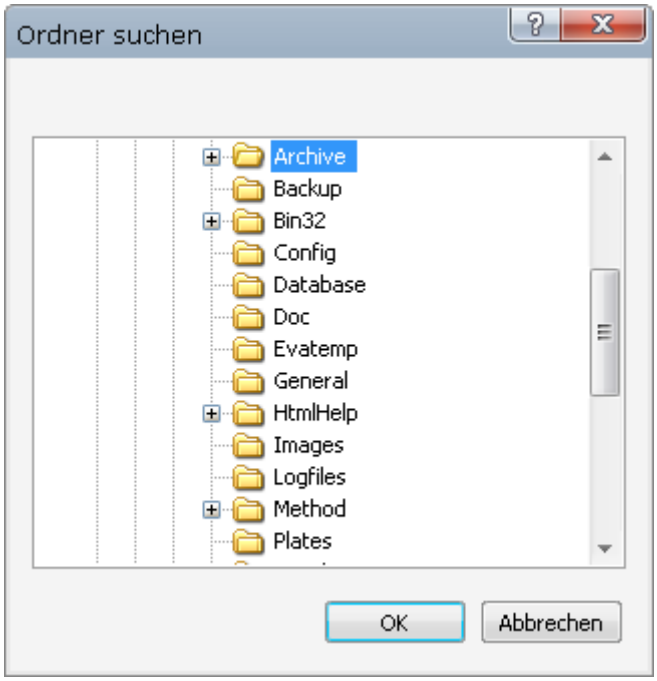
18.1 Export Methods

Methods are stored from the sub-module Method Development. At first, the method to store should be selected. In the pull-down menu *Method* is a function called *Export Method*...



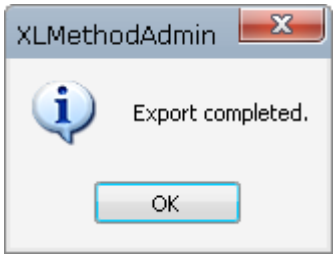
This function opens a box to select the directory for the data storage. To change the directory double-click on the corresponding drive or directory.

The name of the method is used automatically as name of this new subdirectory.



If the method was stored before (the directory still exists), a message will inform you before overwriting the old export files.

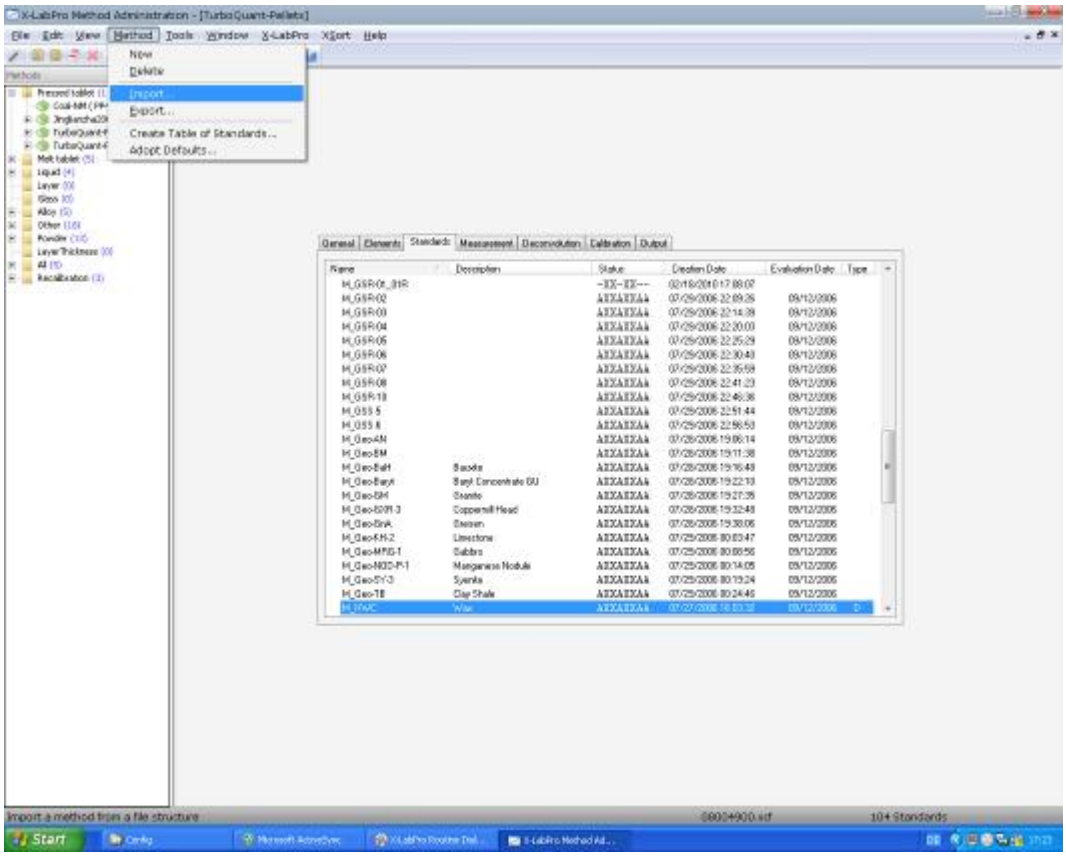
The progress of storing (e.g. the just stored sample) is shown on the screen and at the end of the archiving a message box is shown.



18.2 Import Methods

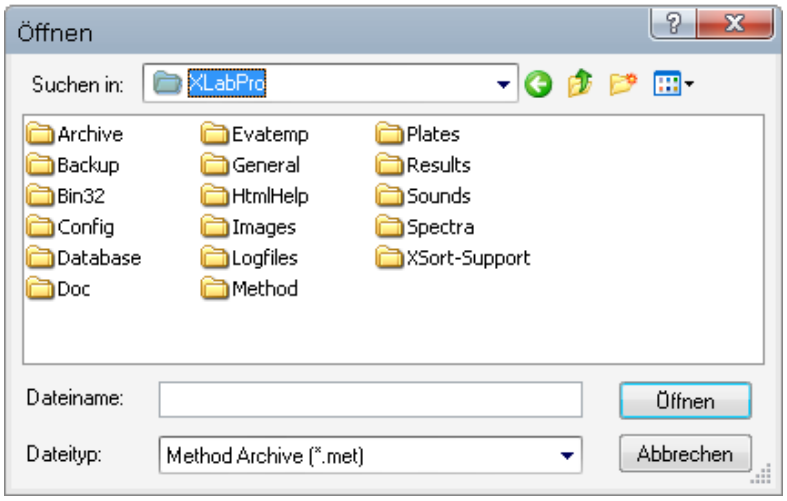
In the X-Lab[Pro] software only the methods in the database structure can be used. Therefore, methods can be exported (for data storage or to transfer methods to other computers) and imported.

To load a method into the database the sub-module *Method Administration* has to be selected. In the pull-down menu *Method* is a function *Import Method*... to load a method.



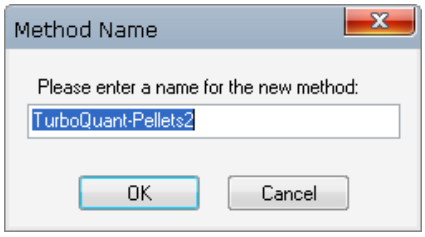
In the following selection box the method archive file (with the extension .mar if using software version 2.5 or older) of the specific method has to be selected. This method archive file is generated automatically when a method is stored. It contains a list of all samples that are part of this method. Without this .mar file, the method can not be restored.

In the line above the selection field, the just selected directory is shown.
To change this directory, a double-click on the target directory is necessary.

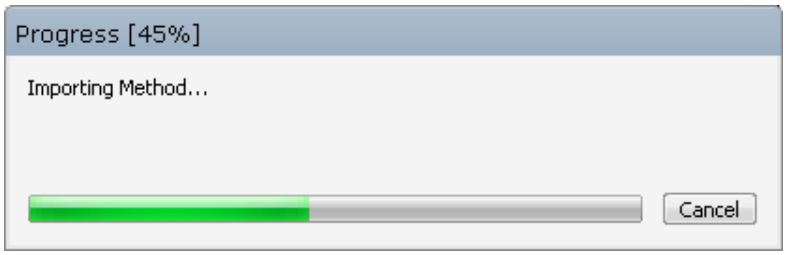


When the directory is selected, only the methodname.mar file will be shown. This file should be selected and the selection confirmed by *OK*.

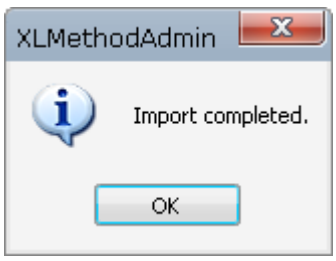
In the next window the name for the method can be modified. The default name is the old name of the method.
The software needs unique method names: If the name of the method already exists, please rename the new method.



After the confirmation or modification of the Method Name, the files will be loaded. The progress of this task is shown in a message box.

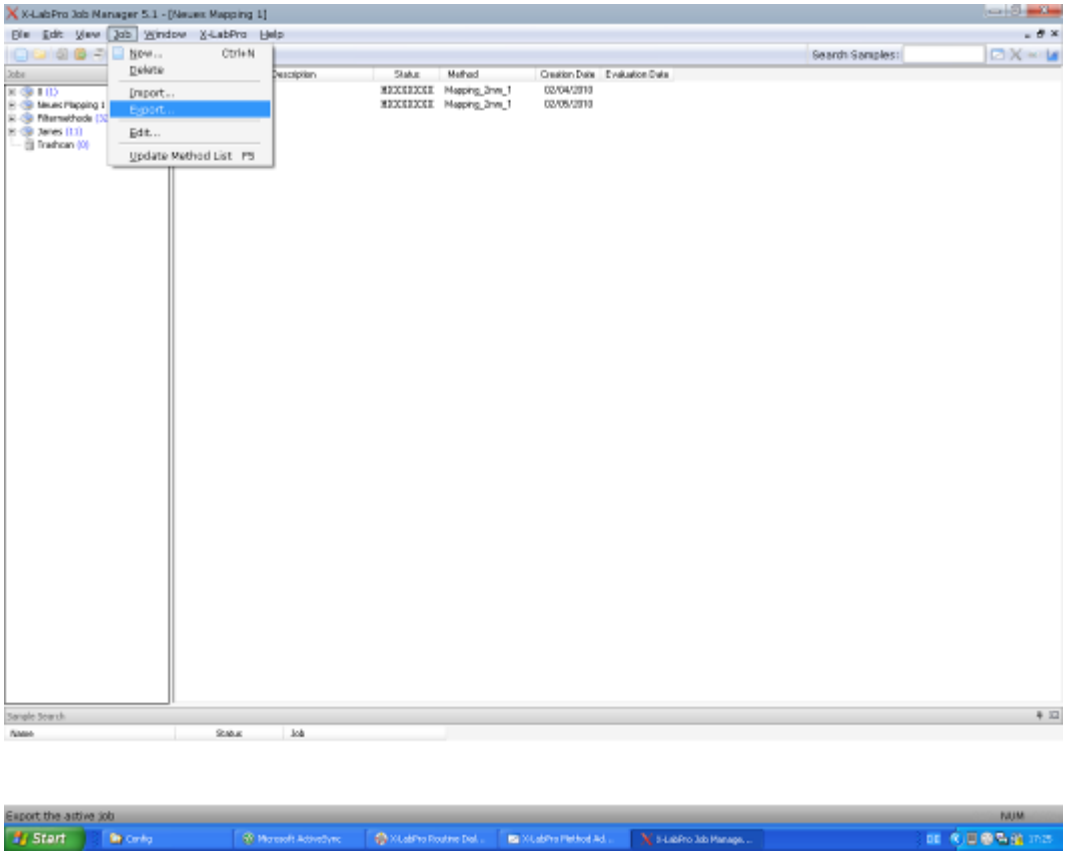


The end of the restoring procedure is displayed in a message box.



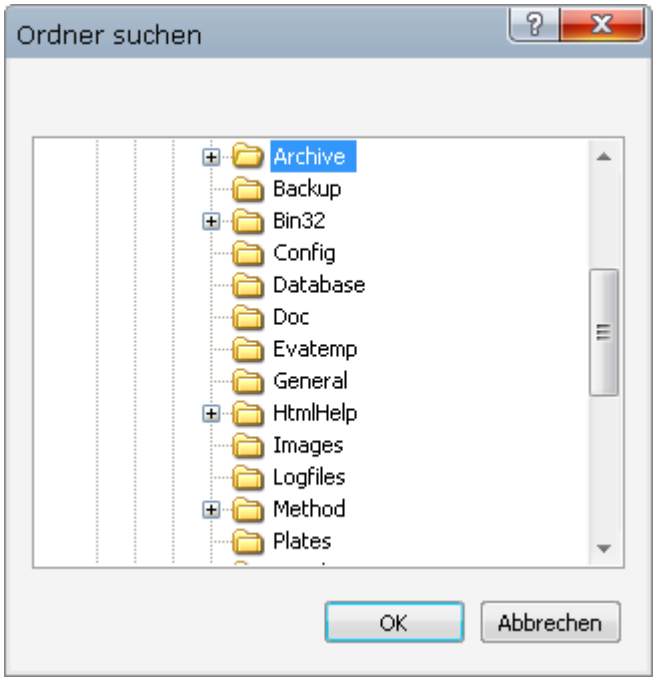
18.3 Export Jobs

Jobs are stored from the submodule *Job Manager*. The job to store must be selected and then the function *Export*... from the pull-down menu *Job* must be activated.

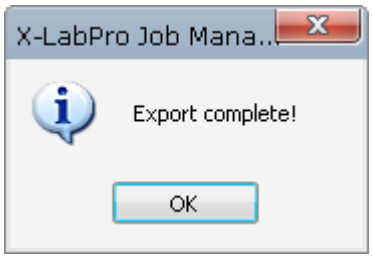


A selection box opens to choose the target directory. The software is automatically creating a subdirectory, so only the directory to store all jobs should be selected. The default setting is the archive subdirectory in the program directory (X-Lab^{Pro}).

The selected directory is shown above the selection window. To change the directory, double-click on the corresponding drive or directory.

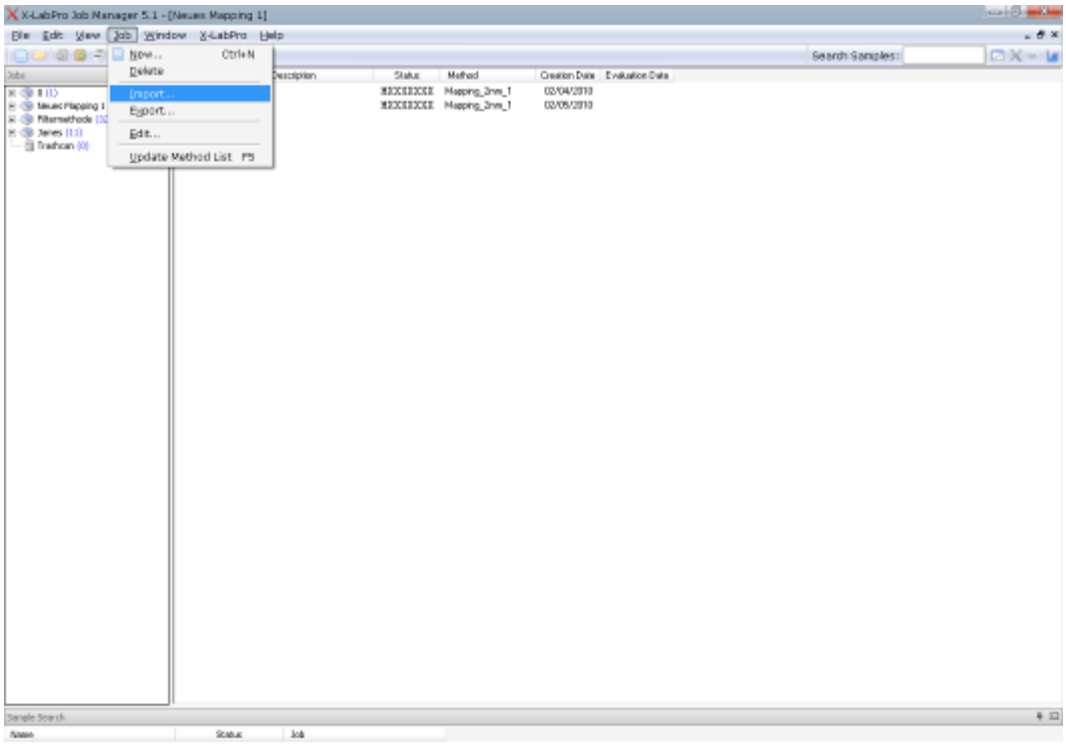


The selection of a specific directory is confirmed by clicking on the OK button. The completed storage is indicated by a message box.

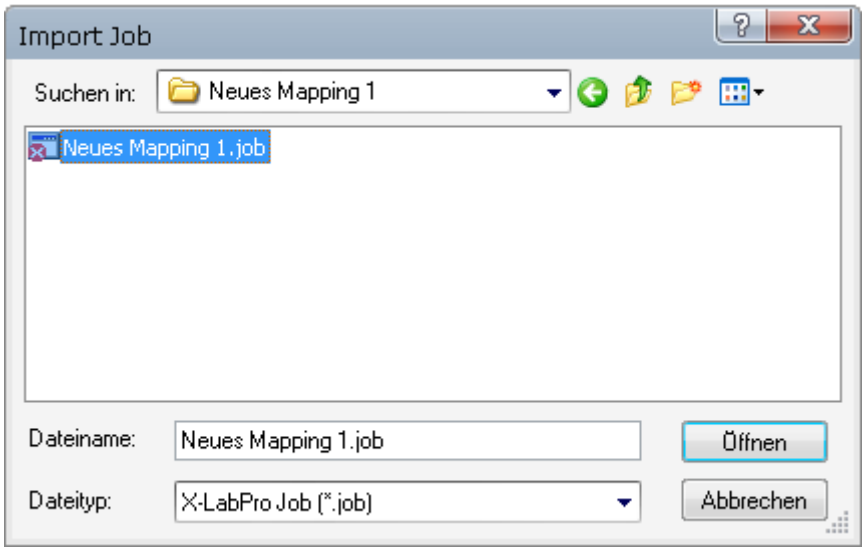


18.4 Import Jobs

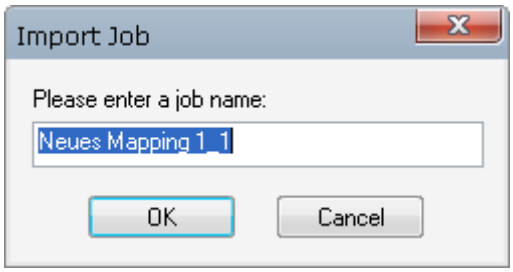
To reload archived jobs, the function *Import*... from the pull-down menu *Job* must be selected.



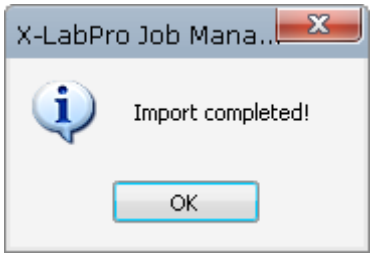
The following selection box shows the subdirectory where the samples are archived. If the directory is correct, this path has to be confirmed.



After selecting a Job, there's the possiblity to change the name of the re-imported job.



A message box shows the end of the restoring process.

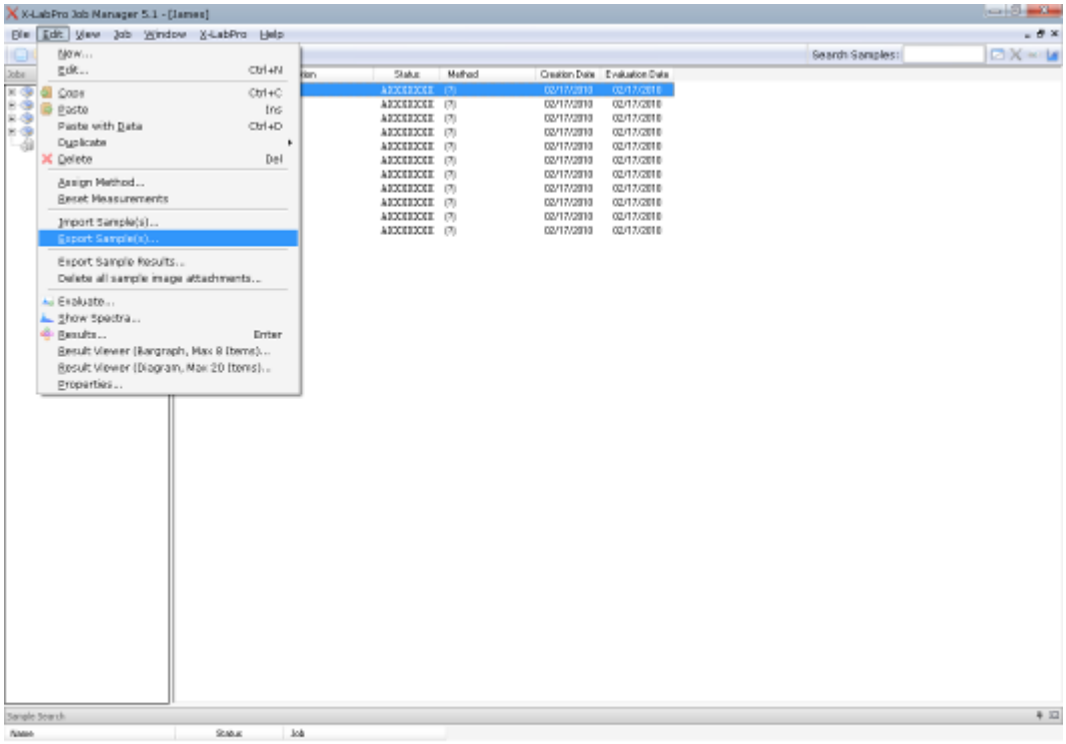


The samples are restored automatically. It is essential that the *Method* that was used for the samples still exists.

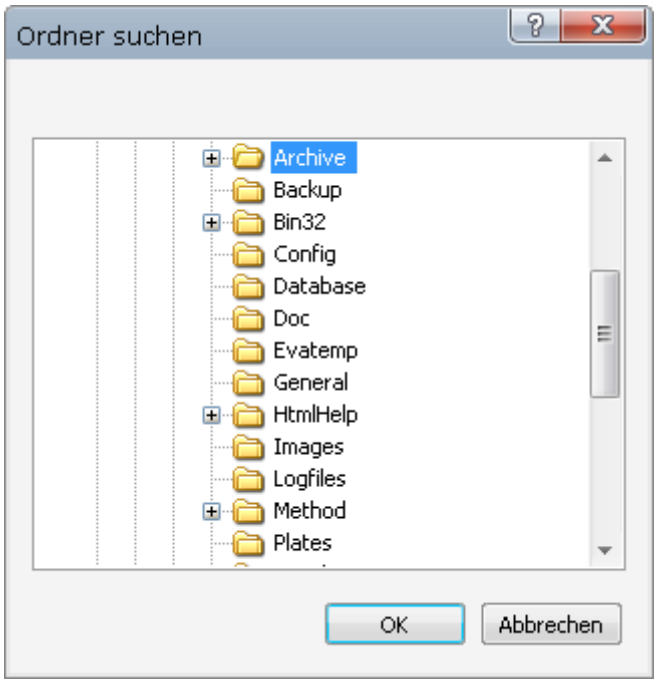
18.5 Export Samples

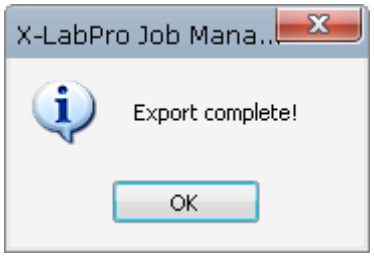
Sometimes it is necessary to export single samples instead of entire methods or jobs; e.g. to transfer them to another computer or to transmit them to Spectro or just to store them. In addition to the *Store Job* and *Store Method* functions the software offers the *Export (Standard) Samples*... function in the submodules *Job Manager* and *Method Administration*.

The samples must be selected. To export the selected samples the function *Export (Standard) Samples*... from the pull-down menu *Job* (or *Method*) has to be selected.



In the following box the sub-directory for the stored samples can be selected. The default sub-directory for exporting samples is Xlabpro\Archive. After the first data exchange, the last used directory will be the default for the next action.



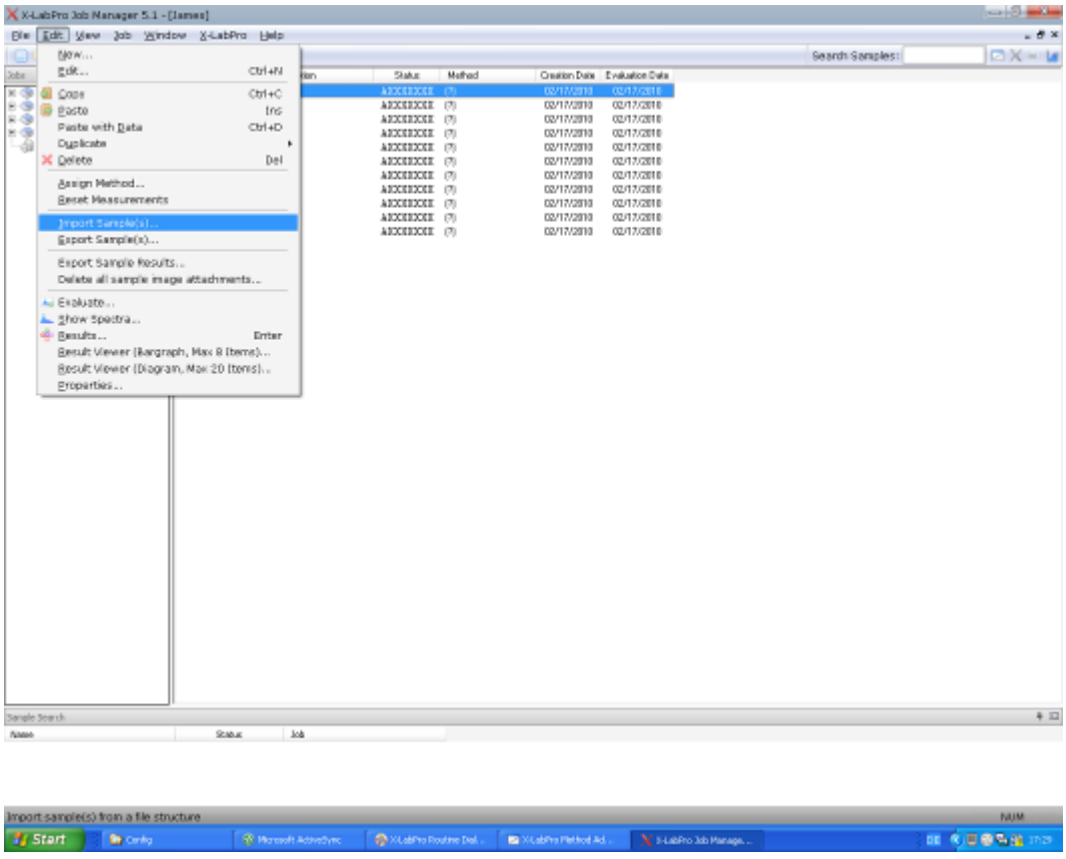


18.6 Import Samples

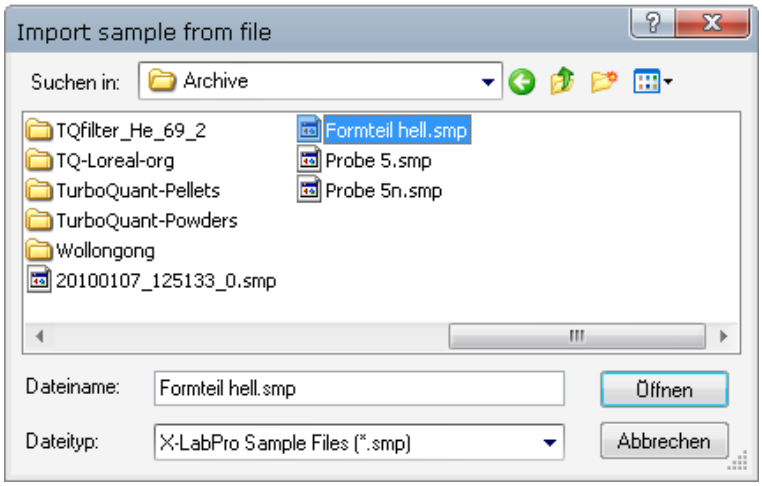
Samples can be imported into the database structure even without being part of a stored *Job* or *Method*. It is possible to load samples into *Jobs* or *Methods* by quite similar procedures.

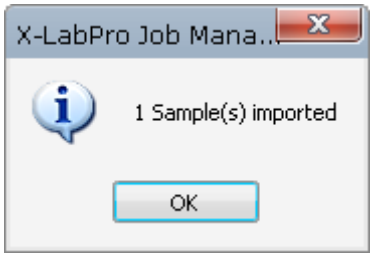
At first the method (or job) in which the samples should be imported must be selected.
The following example is demonstrating the import of samples as standards to an existing method.

In the pull-down menu *Edit* the function *Import (Standard) Samples*... must be selected.



After selecting the directory, a sample (or samples) can be selected.





When samples are imported it is necessary to select the dilution material (if necessary) for the samples.

18.7 Protocol File for Recalibrations

During a Global Recalibration a protocol file is created. This allows to check whether the recalibration was successful and logical!

Hints to control the calculated factors:

- The factors should be around 1.000. Please check, if the range of these factors is between 0.90 and 1.10 (that means 10 % difference to 1.000) and no factor like 1,234.5 is calculated (because a wrong sample was used...).
- The run of the curve of the factors against the atomic numbers should be controlled, whether jumps or discontinuities occur. The only known discontinuity is for the HOPG target between the elements Chlorine and Potassium.
- The heavier the neighbouring elements the smaller is the difference of their factors. Especially for elements heavier than Iron (Atomic Number > 26), there is very often only one factor for the whole sub-measurement (Target). For each target the average and the standard deviation for all factors are calculated at the end of the summary.
  If the standard deviation for the Average Target Value is small enough, one "Target-factor" is used instead of individual factors.

In the following, a part of this document is shown:

```
================================================================
  Global Recalibration
================================================================
    Date/Time: 25.11.2003, 14:36
    Instrument Number: Spectro
    Customer Name: Dr. Oliver Genkel
================================================================

================================================================
  Target Position: 1 (Barkla Scatter, HOPG)
================================================================
    Sample        Z        Old Int.      New Int.      Ratio
================================================================
    MCACAL_0      12        370,456       375,697      0,9860
    MCACAL_0      20        551,782       551,451      1,0006
    MCACAL_0      23        660,381       668,864      0,9873
----------------------------------------------------------------
    MON A_01      12        325,305       320,829      1,0140
    MON A_01      14       3346,442      3338,880      1,0023
    MON A_01      15       2625,216      2625,216      1,0000
----------------------------------------------------------------
    MON B_01      11        123,196       123,196      1,0000
    MON B_01      13       1714,038      1714,038      1,0000
    MON B_01      14        946,172       948,320      0,9977
    MON B_01      20        670,969       671,372      0,9994
    MON B_01      22        694,437       703,162      0,9876
================================================================

    Summary:
    --------

    Z = 11   :  1,0000
    Z = 12   :  1,0000 ±  0,0022
    Z = 13   :  1,0000
    Z = 14   :  1,0000 ±  0,0007
    Z = 15   :  1,0000
    Z = 20   :  1,0000 ±  0,0018
    Z = 22   :  0,9876
    Z = 23   :  0,9873

    Number of Elements:   8
    Average Target Value:  0,9969 ±  0,0058

Extrapolation
 Z = 16   Value:  0,9843
 Z = 17   Value:  0,9881
 Z = 19   Value:  0,9964
 Z = 24   Value:  0,9966
 Z = 25   Value:  0,9966
 Z = 26   Value:  0,9966
 Z = 27   Value:  0,9966
 Z = 28   Value:  0,9966
 Z = 29   Value:  1,0044
 Z = 30   Value:  1,0044
 Z = 31   Value:  1,0078
 Z = 32   Value:  1,0128
 Z = 33   Value:  1,0126
 Z = 34   Value:  0,9994
 Z = 35   Value:  0,9856
 Z = 37   Value:  0,9884
 Z = 38   Value:  0,9872
 Z = 39   Value:  0,9836
 Z = 40   Value:  0,9811
 Z = 41   Value:  0,9826
 Z = 42   Value:  0,9841
 Z = 47   Value:  0,9924
 Z = 48   Value:  0,9942
 Z = 49   Value:  0,9961
 Z = 50   Value:  0,9980
 Z = 51   Value:  0,9999
 Z = 52   Value:  1,0006
 Z = 53   Value:  0,9997
 Z = 55   Value:  0,9980
 Z = 56   Value:  0,9971
 Z = 57   Value:  0,9968
 Z = 58   Value:  0,9967
 Z = 73   Value:  0,9887
 Z = 74   Value:  0,9881
 Z = 82   Value:  0,9847
 Z = 83   Value:  0,9857


================================================================
  Target Position: 2 (Compton/Secondary, Molybdenum)
================================================================
    Sample        Z        Old Int.      New Int.      Ratio
================================================================
    MCACAL_0     INC        703,752       658,966      1,0680
    MCACAL_0     COH        736,582       737,443      0,9988
    MCACAL_0     Ratio        0,955         0,894      1,0692
    MCACAL_0      26       3607,788      3595,518      1,0034
    MCACAL_0      30       3957,655      3980,681      0,9942
    MCACAL_0      33       3466,630      3518,770      0,9852
    MCACAL_0      39       2117,359      2331,336      0,9082
----------------------------------------------------------------
    MON A_01     INC        812,249       836,656      0,9708
    MON A_01     COH        815,117       811,170      1,0049
    MON A_01     Ratio        0,996         1,031      0,9661
    MON A_01      74       3836,704      3793,907      1,0113
    MON A_01      82       4686,778      4581,304      1,0230
----------------------------------------------------------------
    MON B_01     INC       1541,632      1594,764      0,9667
    MON B_01     COH        917,663       920,604      0,9968
    MON B_01     Ratio        1,680         1,732      0,9698
    MON B_01      24        279,201       278,251      1,0034
    MON B_01      28       2263,511      2256,333      1,0032
================================================================

    Summary:
    --------

    Z = 24   :  1,0034
    Z = 26   :  1,0034
    Z = 28   :  1,0032
    Z = 30   :  0,9942
    Z = 33   :  0,9852
    Z = 39   :  0,9082
    Z = 74   :  1,0113
    Z = 82   :  1,0230
  Compton(1) :  1,0018 ±  0,0573
  Rayleigh(1):  1,0002 ±  0,0042

    Number of Elements:   8
    Average Target Value:  0,9915 ±  0,0354

Extrapolation
 Z = 22   Value:  1,0000
 Z = 23   Value:  1,0000
 Z = 25   Value:  1,0000
 Z = 27   Value:  0,9999
 Z = 29   Value:  0,9995
 Z = 31   Value:  0,9983
 Z = 32   Value:  0,9980
 Z = 34   Value:  0,9900
 Z = 35   Value:  0,9718
 Z = 37   Value:  0,9338
 Z = 38   Value:  0,9139
 Z = 40   Value:  0,8933
 Z = 72   Value:  0,9995
 Z = 73   Value:  0,9994
 Z = 78   Value:  0,9982
 Z = 79   Value:  0,9981
 Z = 80   Value:  0,9979
 Z = 81   Value:  0,9978
 Z = 83   Value:  0,9999
 Z = 90   Value:  0,9449
 Z = 92   Value:  0,9281
```

19 Literature

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J. H. Hubbell, W. J. Veigele, E. A. Briggs, R. T. Brown, D. T. Cromer, R. J. Howerton, *Atomic Form Factors, Incoherent Scattering Functions, and Photon Scattering Cross Sections*, J. Phys. Chem. Ref. Data, Vol. 4, No. 3 (1975).

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K. Norrish and J.T. Hutton, An accurate X-ray spectrographic method for the analysis of a wide range of geological samples, Geochim. Cosmochim Acta 33, 431 (1969).

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Spectro Midex Easy GUI

20 How to start

To start the **X-Lab^{Pro} Easy Routine Dialog** right-click on the *Communication Server* symbol. In the upcoming menu select *Easy Routine Dialog*.

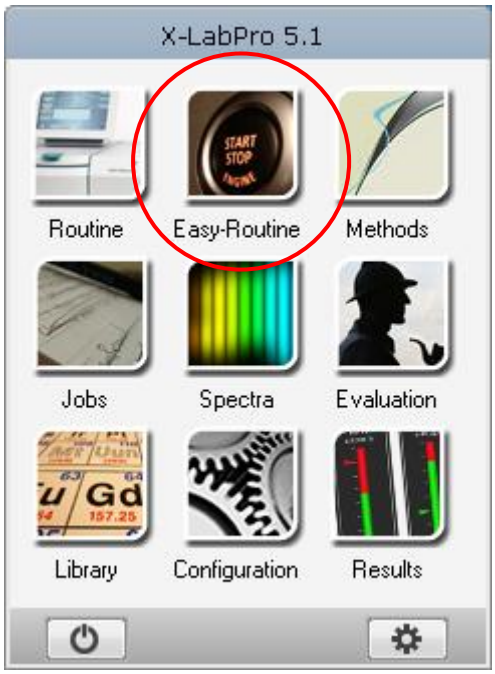


Figure 1: Using the ComServer

21 Starting up

21.1 Log in

When the **Easy Routine dialog** starts up, first you have to provide your login and password.

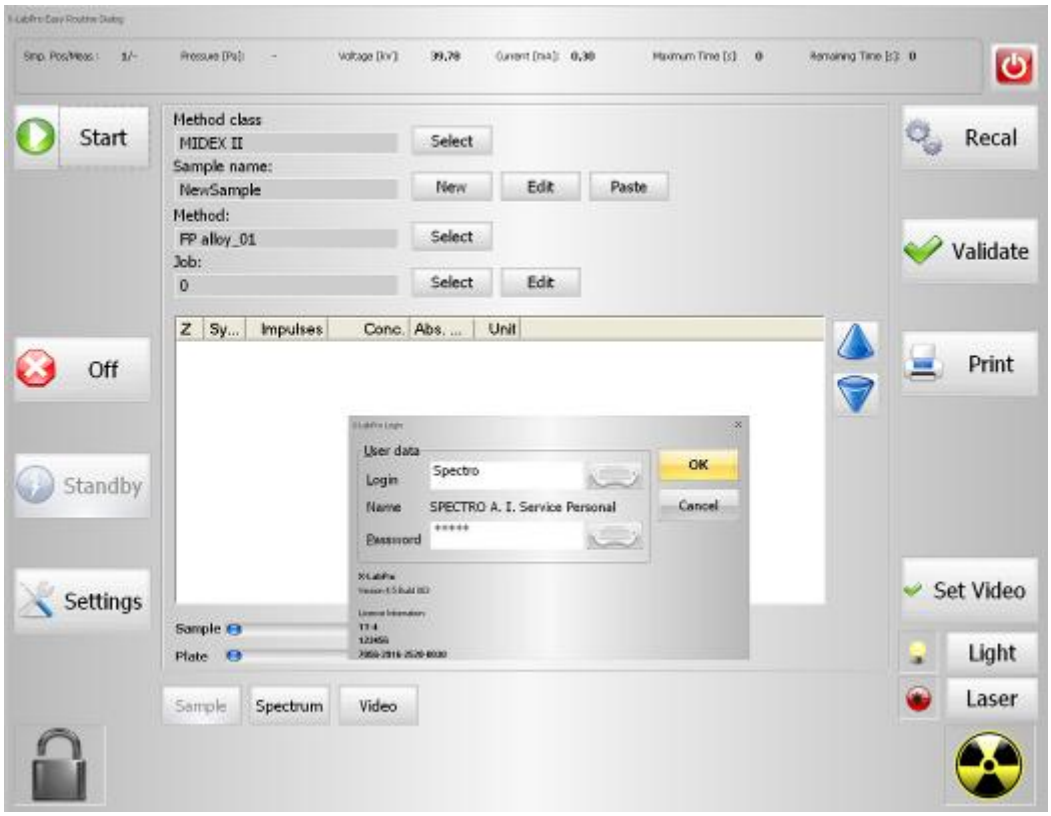


Figure 2: Log in

21.2 Standby mode

As next you are asked whether to go into standby mode. If you do not want to go into standby mode right now, you can switch it on later by using the *Standby button*.

22 Using Easy Routine

22.1 Introducing the dialog

When the start up procedure is finished the dialog will look like in Figure 3.

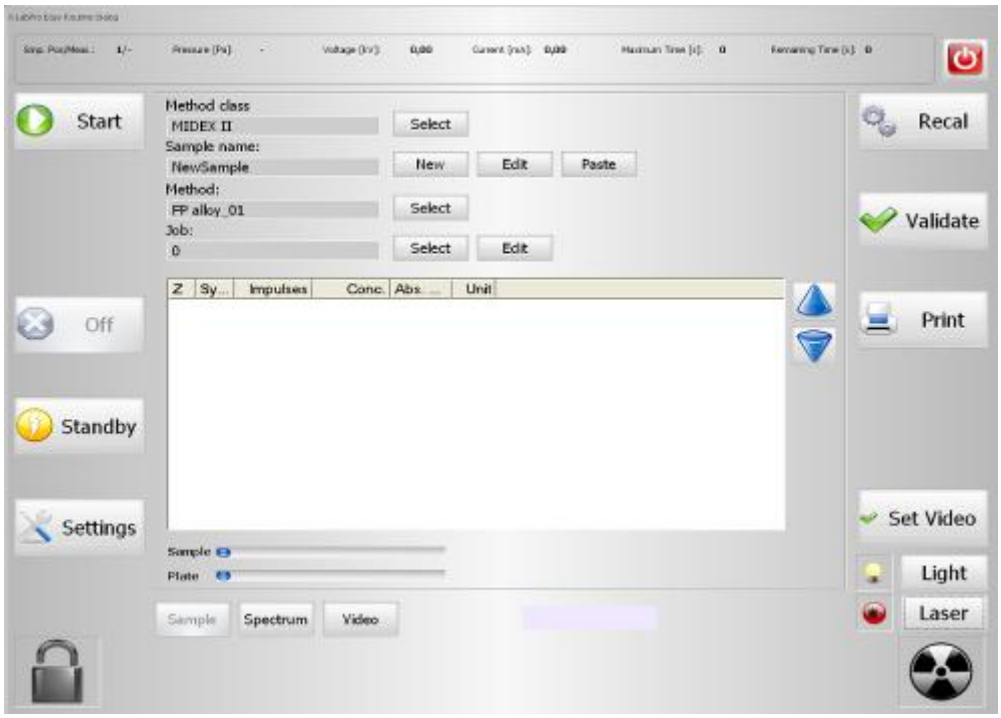


Figure 3: Easy Routine Dialog

In the upper part of the main dialog you can see the *Parameter Bar* stating the actual measurement parameters. While measuring, the bar will be updated continually.

Right next to the *Parameter Bar* is the *Close Button*.

On both sides of the dialog are several *Function Buttons*.

Below the buttons are three *State Icons*.

In the center you can see the *Sample View*. The *Sample View* is shown by default on start up. By using the buttons below the center view you can switch between *Sample View, Spectrum View and Video*.

While measuring the *Spectrum View* shows the measured spectrum.

After a measurement is completed the *Sample View* shows the analysis results.

Video shows a live picture of the measured sample to adjust the manual sample table.

22.1.1 Sample view

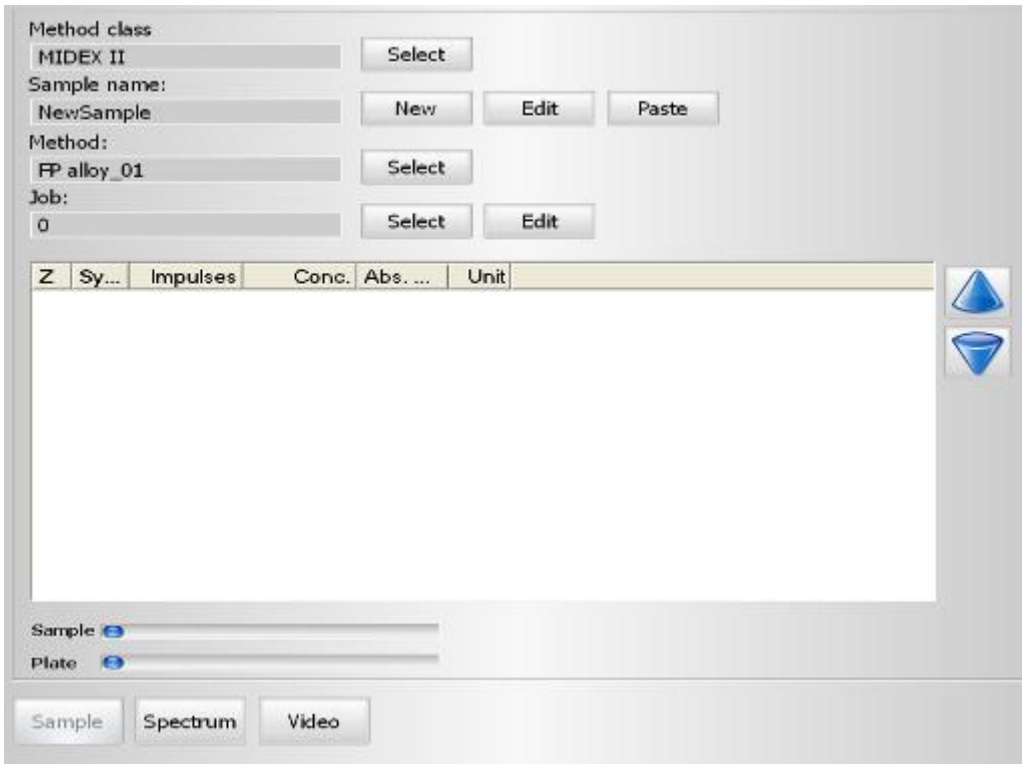


Figure 4: Sample View

The *Sample View* contains all needed controls to prepare a measurement.

In the first four rows you can edit the sample name and select the method class, method and job.

Below is the *Result List* where the measurement results are shown. After performing a *Validation* the list contains an additional row with the validation result.

The progress controls show the remaining measurement time; separated into

- Sample time: the time remaining for measuring the current sample.
- Plate time: the time remaining for the complete measuring process (incl. time for preparing a measurement with gas flush or vacuum).

The two buttons below let you switch between *Sample View* and *Spectrum View*.

22.1.2 Selecting a Method class

Press the *Select button* next to the edit field. A dialog (*Figure 5*) opens and you can select the desired method class.

22.1.3 Selecting a Method

Press the *Select button* next to the edit field. A dialog (*Figure 5*) opens and you can select the desired method.

The dialog only shows methods which are in the current method class.

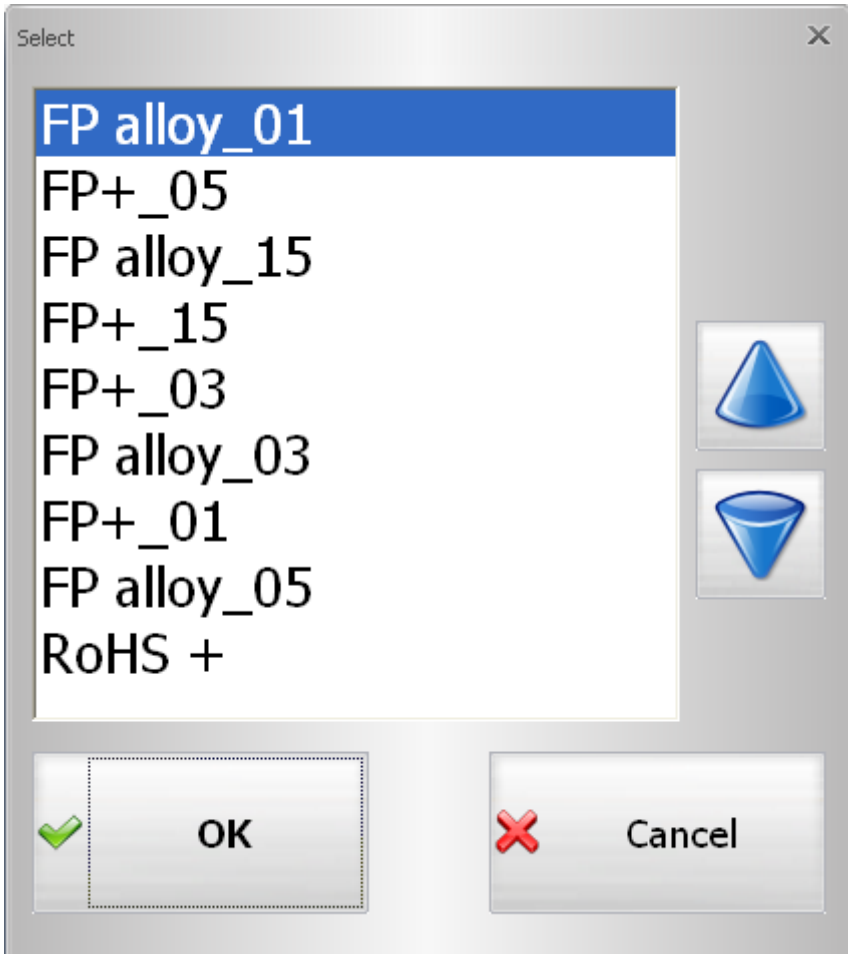


Figure 5: Select dialog

22.1.3.1 Selecting a Job

At start up the job is preset according to the setting from the Configuration Editor.

To select a different job press the *Select button* next to the edit field. A dialog (*Figure 5*) opens and you can select the desired job.

22.1.3.2 Editing a Job

To edit the job press the *Edit button* next to the edit field. A *Virtual Keyboard* (*Figure 6*) appears. Type in the new job and press OK to accept it.

22.1.3.3 Editing the sample name

At start up the sample name is preset with 'NewSample'.

To edit the sample name press the *Edit button* next to the edit field. A *Virtual Keyboard* (*Figure 6*) appears. Type in the new sample name and press OK to accept it.

22.1.3.4 Pasting a sample

Click here, to paste a sample from the *Job Manager* into **Easy Routine Dialog**.

It is not possible to paste a standard. For pasting standards, please use the **Routine Dialog**. Further on, the method to which the sample belongs must not be hidden or finalized.

It is possible to resume the measurement of a not completely measured sample. For example: if your sample contains 6 measurements and 5 of these are already measured, you can paste the sample and start measuring the last one.

It is not possible to paste a completely measured sample.

22.1.3.5 Using the virtual keyboard

Figure 6: Virtual keyboard

The *Virtual Keyboard* can be used like a normal keyboard. *Shift* and *Caps Lock* work in the expected way. Selecting characters with *Shift* is not possible.

To move the cursor in the edit field use the *Arrow buttons* left to the edit field.

To delete the character left to the cursor use the *Delete button* on the right side of the edit field.

Press *OK* to accept the name or *Cancel* to close the dialog.

22.1.4 Spectrum view

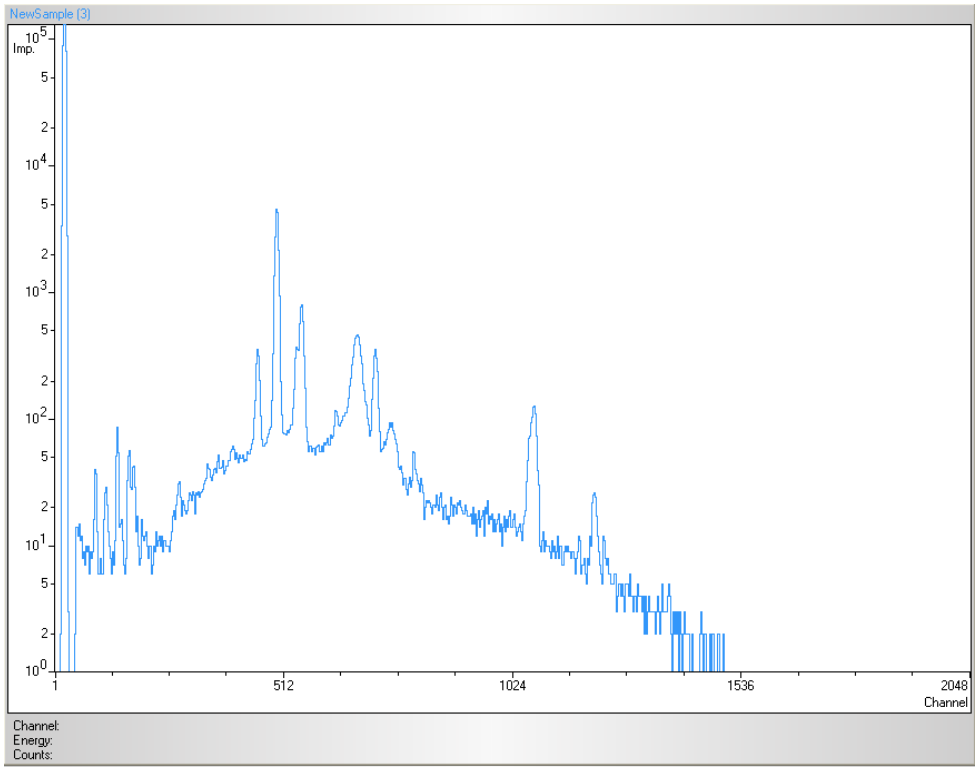


Figure 7: Spectrum View

During a measurement the *Spectrum View* displays the currently measured spectrum.

The *Spectrum View* can be enabled / disabled in the *Settings dialog*.

22.1.5 Close Button

Figure 8: Close button

Clicking the *Close button* exits the **Easy Routine Dialog**. You will have to confirm exiting. If the high voltage is switched on, it will be powered down before the dialog is closed.

22.2 Function Buttons

22.2.1.1 Start

Figure 9: Start button

The *Start button* is active only when no measurement is performed.

Clicking the *Start button* starts a new measurement.

It will change into the *Stop button* while measuring.

22.2.1.2 Stop

Figure 10: Stop button

The *Stop button* appears only during measurements.

Clicking the *Stop button* stops the actual measurement. The high voltage will stay switched on. When the measurement is stopped, the *Start button* is shown again.

22.2.1.3 Off

Figure 11: Off button

The *Off button* is active only when the x-ray tube is on.

Clicking the *Off button* ends the **Standby mode**.

22.2.1.4 Standby

Figure 12: Standby button

The *Standby button* is active only when the x-ray tube is off.

Clicking the *Standby button* switches the instrument into **Standby mode**.

22.2.1.5 Settings

Figure 13: Settings button

The *Settings button* is active only when no measurement is performed.

Clicking the *Settings button* opens the *Settings dialog* (see chapter **Settings dialog** for more details).

22.2.1.6 Recalibration

Figure 14: Recalibration button

The *Recalibration button* is active only when no measurement is performed.

Clicking the *Recalibration button* opens the *Recalibration dialog* (see chapter **Recalibration dialog** for more details).

22.2.1.7 Validate

Figure 15: Validate button

The *Validate button* is active only when no measurement is performed.

Clicking the *Validate button* to prepare a validation. In the upcoming dialog you have to select which method contains the needed *Validation Sample*. After successfully selecting the method, click *Start* to perform the validation.

22.2.1.8 Print

Figure 16: Print button

The *Print button* is active only when no measurement is performed.

Clicking the *Print button* will print the actual measurement results directly to the default printer. When no results are present nothing is printed.

22.2.2 Set Video

Figure 17: Set Video button

The *Set Video button* helps to adjust different parameters of the video display (Brightness, Contrast, Hue, Saturation), of the crosshair (X-Pos, Y-Pos, Size) and light and laser intensity:

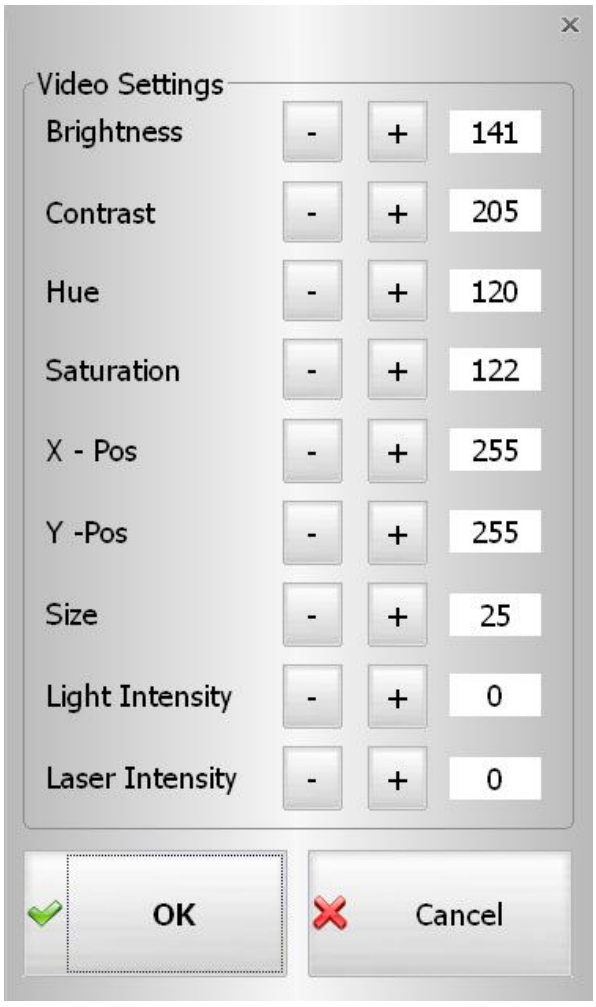


Figure 18: Set Video button

22.2.3 Light

Figure 19: Light button

With the *Light button* the light can be switched on and off.

22.2.4 Laser

Figure 20: Laser button

With the Laser button the laser can be switched on and off.

22.2.5 Parameter Bar

Figure 21: Parameter Bar

The *Parameter bar* states the actual measurement parameters:

- the part measurement of the actual sample.
- the gas flow in liters per hour.
- the voltage in kilovolts.
- the current in milliampere.
- the maximum measurement time for the part measurement of the sample in seconds.
- the measurement time for the part measurement of the sample in seconds.

22.2.6 State Icons

The *State icons* reflect the actual instrument state. Therefore each icon has two different states.

22.2.6.1 Lock/Unlock

Figure 22: Sample chamber locked

The sample chamber is locked.

Figure 23: Sample chamber accessible

The sample chamber is accessible.

22.2.6.2 X-Ray on/off

Figure 24: X-Ray on

The x-ray tube is switched on.

Figure 25: X-Ray off

The x-ray tube is switched off.

22.2.7 Settings dialog

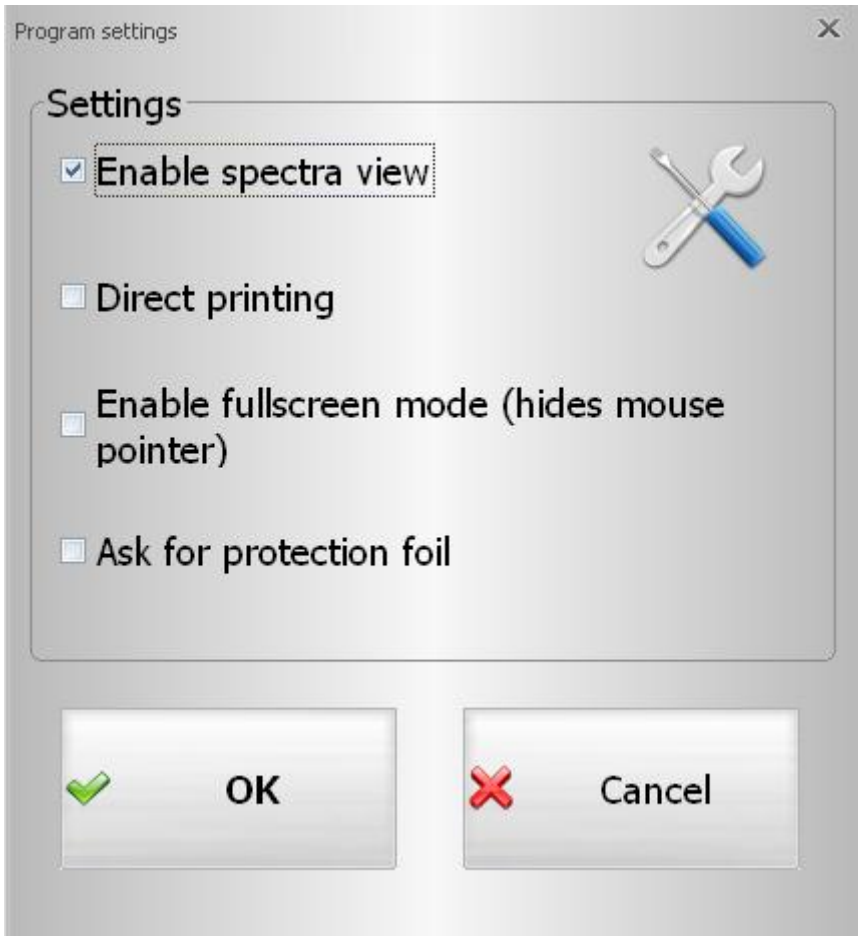


Figure 26: Settings dialog

The *Settings dialog* lets you configure some parts of the **Easy Routine dialog**.

- enable / disable the Spectrum view.
- enable / disable printing directly after evaluation of the measurement.
- enable / disable *Full screen mode*. The *Full screen mode* is suitable only when a touch screen monitor is used because in *Full screen mode* the mouse pointer is hidden.
- enable / disable the question for an inserted protection foil.

22.2.8 Recalibration dialog

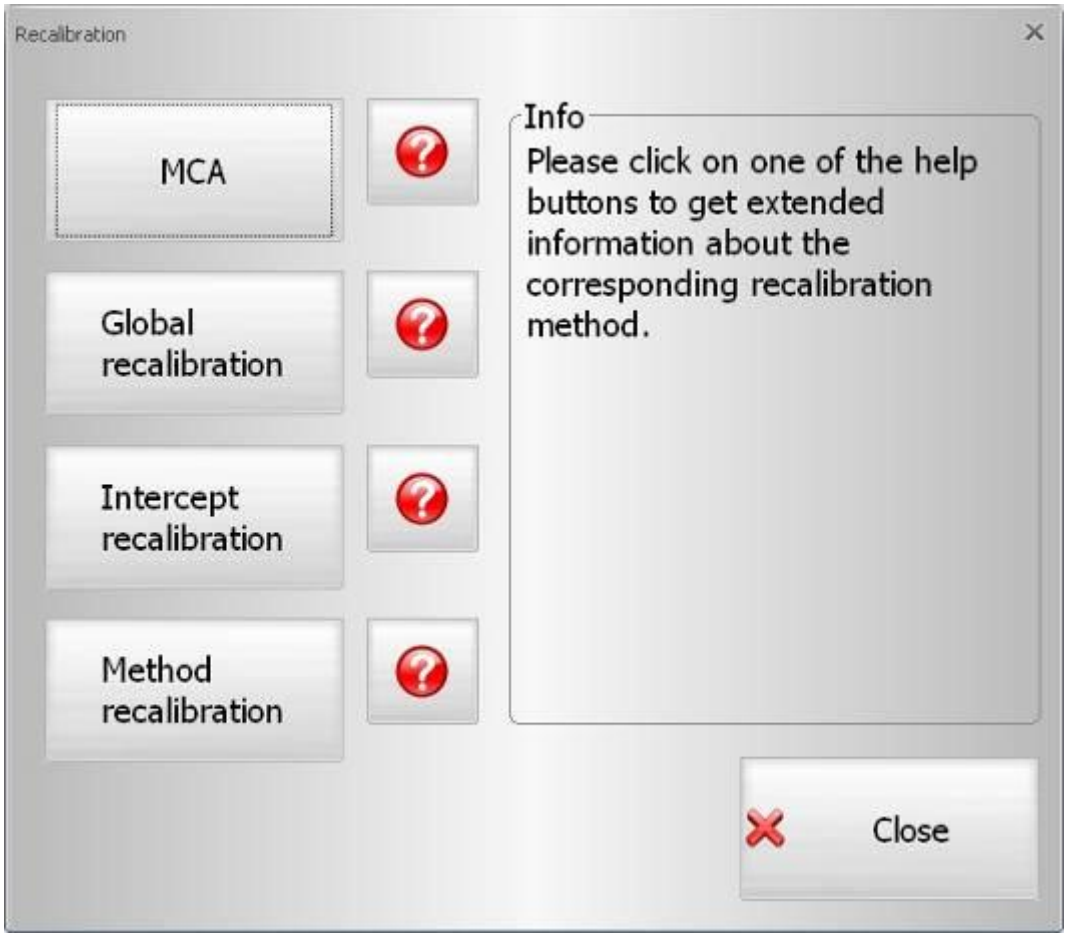


Figure 27: Recalibration dialog

With the *Recalibration dialog* you can prepare the instrument calibration.

Click one of the *Recalibration method buttons* to prepare the recalibration.

For information about the different calibration methods click the *Help button* next to the *Recalibration method button*.

22.3 Recalibration

In this chapter the application flow of the different recalibration methods is explained.

For information about the different calibration methods open *Recalibration dialog* and click the *Help button* next to the *Recalibration method* you are interested in.

22.3.1 MCA

To perform a **MCA Recalibration**, open the *Recalibration dialog* and click the *MCA button*. The recalibration is then prepared. If the actual method does not contain any *MCA sample* you will be noticed.

If a *MCA sample* was found, the **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

When the recalibration is complete the results are shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

22.3.2 Global

To perform a **Global Recalibration**, open the *Recalibration dialog* and click the *Global Recalibration button*. The recalibration is then prepared. If the actual method does not contain any *Global sample* you will be noticed.

If a *Global sample* was found, the **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

Depending on the settings in the **Configuration Editor** the **Global Recalibration** is performed with one or more samples.

If more than one sample is calibrated, a message box advises you when to insert the next sample into the **Sample Chamber**.

When the recalibration is complete the results are shown in the *Result List*. If more than one sample was measured, the results are only written to file and nothing will be shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

22.3.3 Intercept

To perform a **Intercept Recalibration**, open the *Recalibration dialog* and click the *Intercept Recalibration button*. A *Select Dialog* opens and you can choose a method for calibration. The method must contain an *Intercept Sample*. After successfully selecting a method, the recalibration is then prepared.

The **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

Depending on the settings in the **Method Configuration** the **Intercept Recalibration** is performed with one or more samples.

If more than one sample is calibrated, a message box advises you when to insert the next sample into the **Sample Chamber**.

When the recalibration is complete the results are shown in the *Result List*. If more than one sample was measured, the results are only written to file and nothing will be shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

22.3.4 Method

To perform a **Method Recalibration**, open the *Recalibration dialog* and click the *Method Recalibration button*. A *Select Dialog* opens and you can choose a method for calibration. The method must contain a *Method Sample*. After successfully selecting a method, the recalibration is then prepared.

The **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

When the recalibration is complete the results are shown in the *Result List*. In an additional column in the *Result List* the recalibration factors are shown.

The **Easy Routine Dialog** switches back to *Normal Mode*.

22.4 Validation

In this chapter the application flow of the validation is explained.

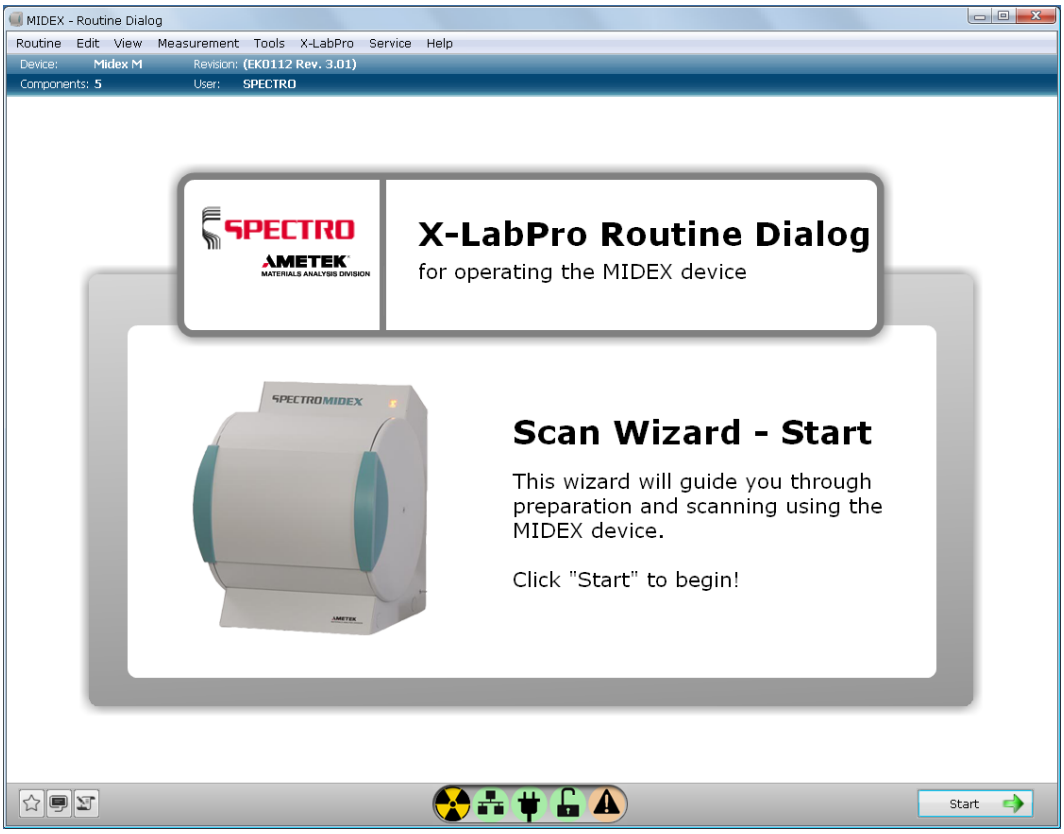
To perform a **Validation**, click the *Validation button*. A *Select Dialog* opens and you can choose a method for validation. The method must contain a *Validation Sample* against which the new sample is validated. After successfully selecting a method, the **Validation** is then started.

When the **Validation** is complete the results are shown in the *Result List*. In an additional column in the *Result List* the validation result is shown:

- a marks a valid result, the measured concentration was within limits.
- a marks an invalid result, the measured concentration was out of range.

The **Easy Routine Dialog** switches back to *Normal Mode*.

SPECTRO MIDEX Tutorials


MIDEX - Routine Dialog
Routine Edit View Measurement Tools X-LabPro Service Help
Device: Midex M Revision: (EK0112 Rev. 3.01)
Components: 5 User: SPECTRO
X-LabPro Routine Dialog
for operating the MIDEX device
Scan Wizard - Start
This wizard will guide you through preparation and scanning using the MIDEX device.
Click "Start" to begin!
Start

23 About this Manual

This manual describes the operation of a MIDEX device. Unlike the older versions of the MIDEX device the new version does not use the common X-Lab[Pro] Routine Dialog for setup and operation. All options and controls appear as the user needs them, not before. This makes it easy to get started using the Spectro MIDEX. Even complex scan scenarios can be configured fast and clear.

Conventions

Throughout this document, a set of typographical conventions is used to define elements and references to the application items. Familiarity with these conventions will help your understanding of the topics covered.

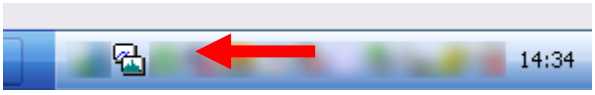
Colored Text	Identifies a text you will find in the current dialog, view or application (e.g. title of a dialog box or the entries of a combo box).
	This symbol is used for a **Note**, for general instructions and advices.
	This symbol is used for a **Tip**, for special instructions for optimal use of the system.
	This symbol is used for a **Warning** (instructions to avoid dangerous situations).

24 Getting started

24.1 Application Requirements

24.1.1 Starting the Application

The Routine Dialog is started through the X-Lab[Pro] Com server application running in the system tray:



Right click the icon to open the X-LabPro application launcher (Com Server) and choose the menu item MIDEX – **Routine Dialog**. This will launch the application and require authorization as first step.

> It is possible to create a shortcut to the application on the desktop. Right click on the desktop and select Create shortcut. Choose C:\XLabPro\Bin32\XLRoutineDlgMII.exe as target path. Then enter Routine Dialog Midex II as shortcut name.

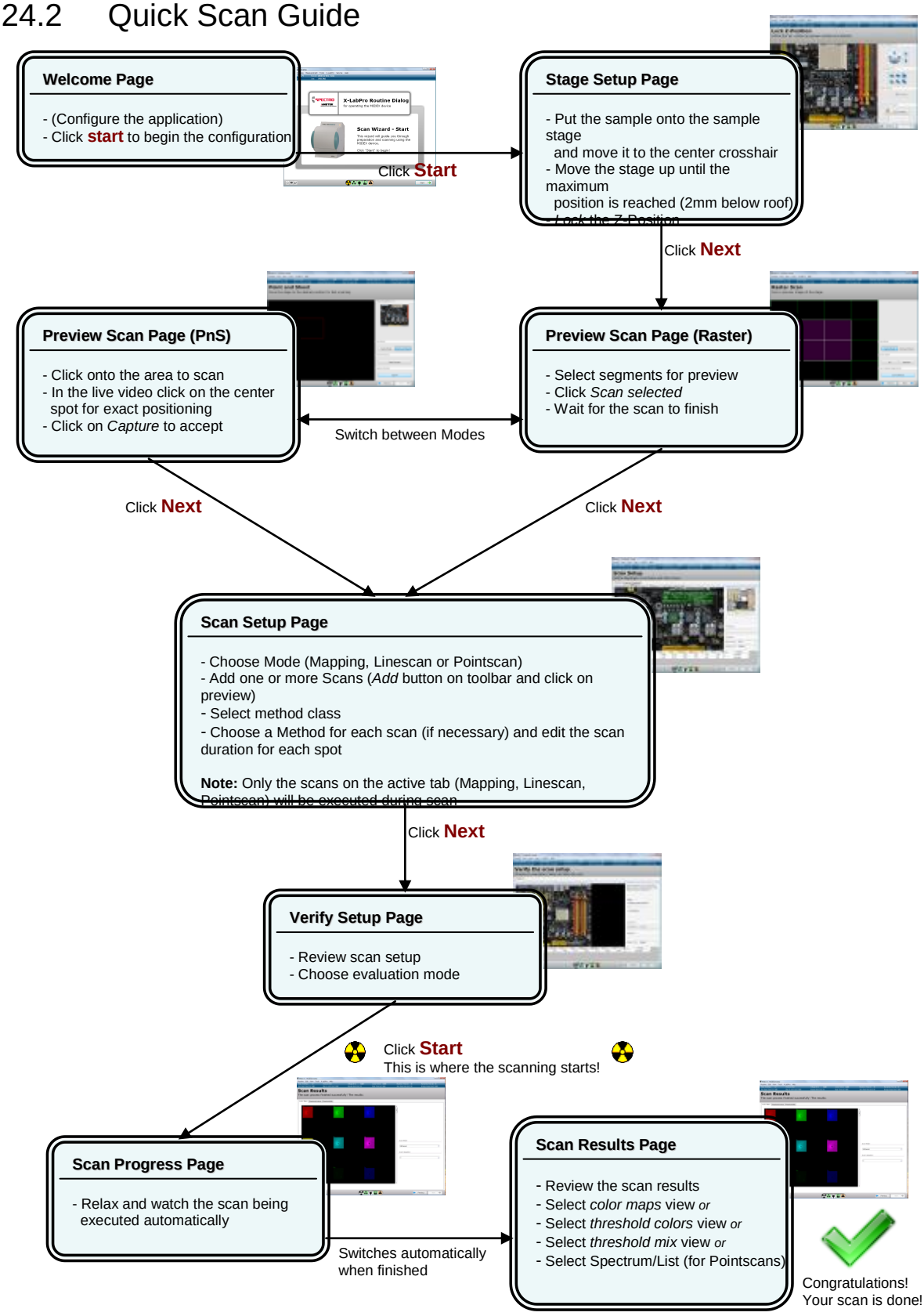
24.1.2 Shutting down the Application

When the Routine Dialog is running the application can be closed like any typical window using the button in the top right corner of the main application window. Another option is to use the main menu of the application (**Routine → Exit**) or the windows taskbar (right click on the window item and select **close**). The application will shut down the device if necessary which can take some time. Review the measurement parameters bar for the shutdown status.

	Never, under any circumstances use the windows task manager to terminate the application process! The high voltage of the device would not be shut down properly.

	In case of an abnormal termination of the application process start the application again. The MIDEX Routine Dialog will detect the device state after launch and shut down the high voltage of the device if needed.

24.2 Quick Scan Guide


Welcome Page
- (Configure the application)
- Click start to begin the configuration
Click Start
Stage Setup Page
- Put the sample onto the sample stage
and move it to the center crosshair
- Move the stage up until the maximum
position is reached (2mm below roof)
- Lock the Z-Position
Click Next
Preview Scan Page (PnS)
- Click onto the area to scan
- In the live video click on the center spot for exact positioning
- Click on Capture to accept
Switch between Modes
Preview Scan Page (Raster)
- Select segments for preview
- Click Scan selected
- Wait for the scan to finish
Click Next
Click Next
Scan Setup Page
- Choose Mode (Mapping, Linescan or Pointscan)
- Add one or more Scans (Add button on toolbar and click on preview)
- Select method class
- Choose a Method for each scan (if necessary) and edit the scan duration for each spot
Note: Only the scans on the active tab (Mapping, Linescan, Pointscan) will be executed during scan
Click Next
Verify Setup Page
- Review scan setup
- Choose evaluation mode
Click Start
This is where the scanning starts!
Scan Progress Page
- Relax and watch the scan being executed automatically
Switches automatically when finished
Scan Results Page
- Review the scan results
- Select color maps view or
- Select threshold colors view or
- Select threshold mix view or
- Select Spectrum/List (for Pointscans)
Congratulations!
Your scan is done!

25 Routine Dialog

The Routine Dialog for the Midex was developed to simplify the scan process. It will assist the user from the beginning at setting up a scan and supports all required actions at the moment they are needed.

25.1 Wizard Style

The user interface of the MIDEX Routine Dialog implements a wizard style workflow. The user is directed through the device setup, scan configuration and scan processes step by step

The process of setting up a scan, scanning and reviewing results can be done in some very easy steps:

- Place the sample onto the stage inside the test chamber
- Move the sample into the center of the camera (using live video)
- Move the sample to the highest possible position and lock it (protects the sample from damaging the detection system)
- Capture a preview image of the sample (combining one or more camera images)
- Select the spots to scan on the preview image
  - Multiple spots, rectangular = **Mapping** or
  - Multiple spots, linear = **Linescan** or
  - Single spots = **Pointscan**
- Select scan method and scan duration
- Start the scan (executes automatically, shows progress)
- Review the scan results (multiple result presentations available)

25.2 Integration into X-Lab^{Pro} 5

The MIDEX Routine Dialog is one component of X-LabPro 5.0.

X-LabPro 5.0 consists of several components used to configure and manage the device and the scan methods, to execute evaluations and to review scan results.

The following table lists all components of X-LabPro 5.0 for use with the MIDEX device. For detailed information or help on the component please consult its Online Help:

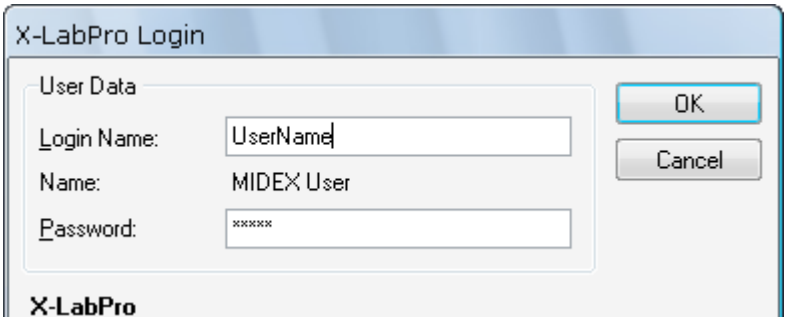
Method Administration	The Method Administration is used to manage and develop scan methods. Methods listed here can be used for scanning using the MIDEX Routine Dialog. See chapter “Method class and method selection” for more information

Job Manager	The Job Manager combines multiple Pointscans to jobs. MIDEX Routine Dialog supports jobs only for Pointscans. Mappings and Linescans use their own archive file format. See chapter "Setup Pointscans" for more information on jobs.
Spectra Viewer	The Spectra Viewer displays results of scans either as spectra, for Mappings and Linescans also as color maps or threshold maps.
Configuration Editor	The Configuration Editor manages all settings of the X-LabPro application and the device.
Library of Atomic Data	This library contains all atomic data for use within the evaluation process.

25.3 Login and Authorization

After starting the application it requires to authorize with X-Lab^{Pro} 5.0. If there is already a component of X-Lab^{Pro} authorized and running, the credentials of that component will be used and no further login is required.

The Log-In dialog will be shown as follows:



User accounts and passwords can be created and edited using the Configuration Editor.

Enter a username and password and click on **OK** to authorize. If the authorization succeeds, the login dialog disappears and the initialization sequence of MIDEX Routine Dialog continues.

If the login details are not correct a message is shown. Click **OK** and try again. Username and password fields are not case sensitive.

If you click on **Cancel** the authorization process will be aborted. In this case the MIDEX Routine Dialog will be closed and the application will shut down.

	MIDEX Routine Dialog cannot be used without authorization!

25.4 Connecting to the Device

After authorizing the application attempts to connect to the MIDEX device connected to your computer. If the system is set up to run in simulation mode a connection will only be simulated (see Chapter 4.2.3 Simulation Mode).

The status of the connection process will be shown in the device control log window (see Chapter 4.3.6 Device Control Log Window). This window is part of the main application window and will automatically pop up until the initialization process finished.

The interface provides a status icon to verify a device was successfully connected and initialized. This status icon is described below in Chapter 4.2.2 Testing the connection.

25.4.1 Connection Setup

To setup a connection the device must be connected to the computer running the MIDEX Routine Dialog application. The connection options can be edited using the Configuration Editor. Please consult the **Configuration Editor** Online Help for more information.

25.4.2 Testing the Connection

There are two ways to verify a successful connection:

- Review the device control log
  The device control log window displays status messages generated during the initialization of the application/device. It lists all instrument components

found and the device connected. If the device was detected the connection was successful.

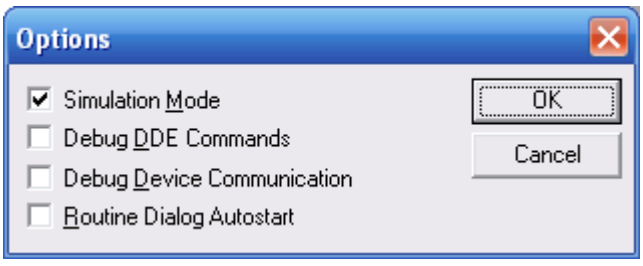
- Notice the status icon in the bottom bar
  The bottom bar of the application window contains several status icons. The second is showing the connection status of the device. The following list shows the meaning of the different status icons:

	The device is connected successfully and ready for use
	A device is not connected or not yet initialized
	The application is busy connecting to the device

	Move the mouse pointer over the status icon and leave it there; a popup window will open and display a notification regarding the current status. Move the mouse pointer outside of the icon and the popup window disappears immediately.

25.4.3 Simulation Mode

Without a connected device the application can still be started. The application has to be started in simulation mode. This setting can be set in the options dialog of the X-LabPro Com Server (launcher in the system tray). Right click on the tray icon and choose **Options**. The following dialog will show up:



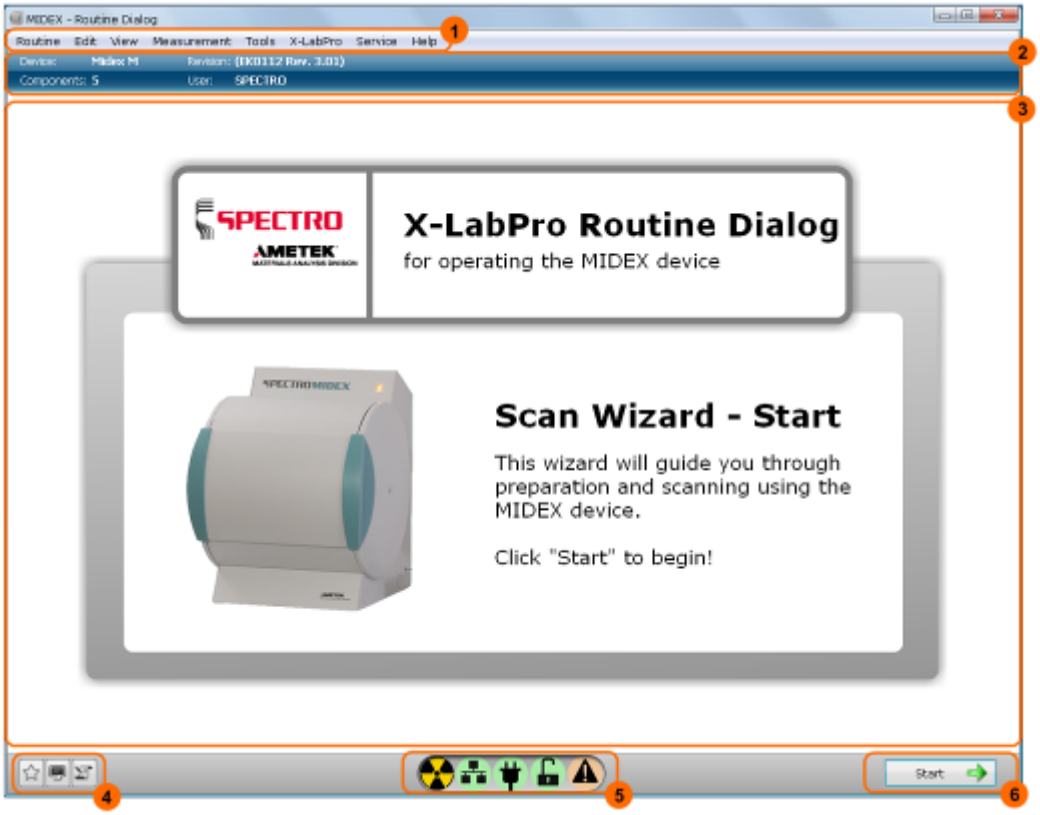
Mark the simulation mode checkbox to enable it. Click OK to save the new setting. This setting will get active when the MIDEX Routine Dialog is restarted.

When started in simulation mode all actions and reactions of the interface are just simulated. The application will not connect to a device, even if it is connected. The last (right) status bar icon shows a simulation mode symbol if it is active:

	Simulation mode is activated

	In simulation mode all spectra generated are simulated and do not contain measurement information!

25.5 Routine Dialog Main Window



1	Main Menu	See chapter 4.3.1
2	Measurement Parameters Bar	See chapter 4.3.2
3	Wizard Page Area	See chapter 4.4
4	Tool Windows Toggle Buttons	See chapter 4.3.5 – 4.3.7

5	Status and Notification Area	See chapter 4.3.3 & 4.3.4
6	Wizard Navigation Area	See chapter 4.3.8

25.5.1 Main Menu Items

The MIDEX Routine Dialog main menu contains general items which are not directly required for device operation. The main menu provides additional functionality like shutting down the application, switching the device on/off, launching this help file, etc.

The following list shows all available menu items and describes their functionality:

Routine	Contains menu items affecting the routine application
------- Exit	Shuts the application down. *If high voltage of the device is active, the routine shuts the device down first. This may take some time. The measurement parameters bar informs about the current state of the device generator values.*
Edit	Contains menu items affecting the data in the Routine Dialog. *Sub items get only active when it is possible to use them.*
------- Paste Standard	Pastes a standard to the Pointscan list on Scan setup Page *(see chapter 4.4.5.11.2)*
View	Switches toolbars/windows and sets view options
------- X-LabPro 5 Bar	Toggles the visibility of the X-Lab^{Pro} Bar *(see chapter 4.3.5)*
------- Device Control	Toggles the tool window for device messages *(see chapter 4.3.6)*
Tools	Device operations and service menu items
------- Instrument Test Window	Allows controlling the device components manually (Supervisor only)
------- Test Measurement	Allows starting a measurement for testing purposes (Supervisor only)
------- Init Sample Stage	Moves the sample stage back to its root position

------- Reload Methods	Reloads the Method buffer and reads newly added methods
------- Switch Instrument Off	Shuts the device down
------- Enter Standby Mode	Activates the standby state of the device (holding voltage)
X-Lab^{Pro}	Contains items to launch other X-Lab^{Pro} components (same items like X-Lab^{Pro} Bar)
------- Method Administration	Launches the Method administration of X-Lab^{Pro}
------- Spectra Viewer	Launches the Spectra Viewer of X-Lab^{Pro}
------- Job Manager	Launches the Job Manager of X-Lab^{Pro}
------- Atomic Library	Launches the Library of atomic data of X-Lab^{Pro}
------- Configuration Editor	Launches the Configuration Editor of X-Lab^{Pro}
------- Evaluation	Launches the Evaluation of X-Lab^{Pro}
------- Routine Help	Opens this Help Manual
Help	Help and information about MIDEX Routine Dialog
------- Help Manual	Opens this manual
------- About MIDEX Routine	Shows a dialog containing application and version information

25.5.2 Measurement Parameters and Information Bar

Below the main menu the interface presents the measurement parameters bar. This bar is always visible and contains essential information about the state of the device and the progress of the measurement.

The following table describes the values shown in the parameters bar:

Smp. Pos/Meas.	Shows the current scan id and sub measurement id (Pointscan only)
Pressure [Pa]	(reserved for use with vacuum option)
Voltage [kV]	Shows the current voltage produced by the X-ray generator
Current [mA]	Shows the current mA value produced by the X-ray generator
Maximum Time [s]	Presents the time span in seconds scheduled for the active scan
Remaining time [s]	Presents the remaining time of the current scan in seconds *(not overall time)*

25.5.3 Status Icons

The bottom bar of the main application window contains 5 bubble icons presenting the current device/application status.

The **first** icon shows the status of the **X-ray** tube. Is the icon grayed out the X-ray generator is not active. The status icon turns yellow when X-ray gets active:

	X-ray is **inactive**
	X-ray is **active**.

The **second** icon displays the connection status to the MIDEX device. If the icon is grayed out there is no device connected:

	There is no device connected *(at least not yet)*
	The application is busy connecting to the MIDEX device.
	The application successfully connected to the MIDEX device

The **third** icon shows the state of the device power supply. The icon will be grayed out if no status was detected. This can happen if the optional UPS (uninterruptible

power supply) is not installed. A UPS is recommended to support a soft shutdown of the x-ray tube if the main power was interrupted.

	The power status of the device could not be detected.
	The main power line was interrupted. The Routine Dialog will shutdown the device safely and close the MIDEX routine dialog application.
	The main power line is connected and supplying the device with power.

The **fourth** icon presents the state of the sample chamber door lock. If the icon is red, the chamber is locked and cannot be opened.

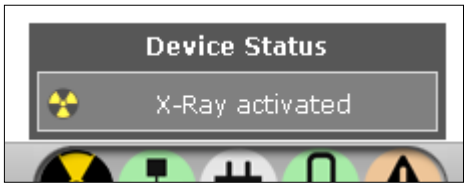
	The chamber door is unlocked and can be opened at any time.
	The door to the chamber is locked and cannot be opened.

The **fifth** and last icon is usually empty (gray). It will change if the application is launched using the simulation mode flag (see 4.2.3). It will also show if the device is transmitting data to the computer or if the detector I regenerating.

	This is the default state of the icon. There is nothing wrong about it.
	The simulation mode is activated. All actions and device responses are only simulated. There is no real device communication.
	The device is busy transmitting data from the device to the computer.
	The detector is regenerating. (not yet used)

25.5.4 Popup Notifications

To clarify the meaning of the displayed status icons the interface provides popup notifications. These notifications appear immediately as you move the mouse pointer over the status icon. If you move the mouse pointer outside of the icon or notification area it will disappear. The notification displays the state of the corresponding icon as simple text. Here are some examples of these notifications:



25.5.5 X-Lab^{Pro} Bar

The bottom bar of the main application window contains 3 buttons which can be used to toggle tool and notification windows. The first button can be used to switch the X-Lab^{Pro} Bar on and off.

The X-Lab^{Pro} Bar lists the commonly used components of X-Lab^{Pro} to make them easy to access from the MIDEX Routine Dialog interface. Available options are:

Method Administration
Spectra Viewer

Job Manager
Library of Atomic Data
Configuration Editor
Evaluation
Help **(for MIDEX Routine Dialog)**

Simply click on the button to launch the corresponding X-LabPro component. As you are already authorized by logging into a MIDEX equipped with xyz stages Routine Dialog it is not required to log into the started component again.

Please note that instead of the buttons in the X-LabPro Bar you can use the X-LabPro menu item in the application main menu.

25.5.6 Device Control Log Window

The bottom bar of the main application window contains three buttons which can be used to toggle tool and notification windows. The second button can be used to switch the device control log window on and off.

Show or hide Device Control Log
Start
Device Control
Device Control Log Window
Clear all log entries
Save the log to a file
Copy the log to the clipboard

The Device Control Log lists all notifications related to the device operation. During connection the device control log window is shown automatically. It will be hidden if the connection process has finished.

On the right side of the window you can find three tool buttons. These buttons can be used to clear the log, save to a file or copy the listed text into the Windows clipboard.

25.5.7 Device Communication Log Window

The bottom bar of the main application window contains 3 buttons which can be used to toggle tool and notification windows. The third button can be used to switch the device communication log window on and off.

This information is required for service purposes only.

25.5.8 Wizard Navigation

The right side of the window bottom bar contains the navigation buttons. These buttons allow switching between the wizard pages.

The button state depends on the current state of the wizard page. For example the process can only advance to the scan setup page if there is a preview image available. Because of that the next button in the preview scan page gets enabled after the preview image was scanned correctly.

The navigation buttons will switch to a special state if the following step executes an action. For example on the setup verification page the next button switches to a **Start** button to clarify that the click on it will launch the scan process.

25.6 Wizard Pages and Device Operation

This chapter will describe the application workflow in detail. Every major step during the scan process is represented by a wizard page. It is easy to navigate back and forth through the steps/pages using the navigation buttons (see chapter 4.3.8)

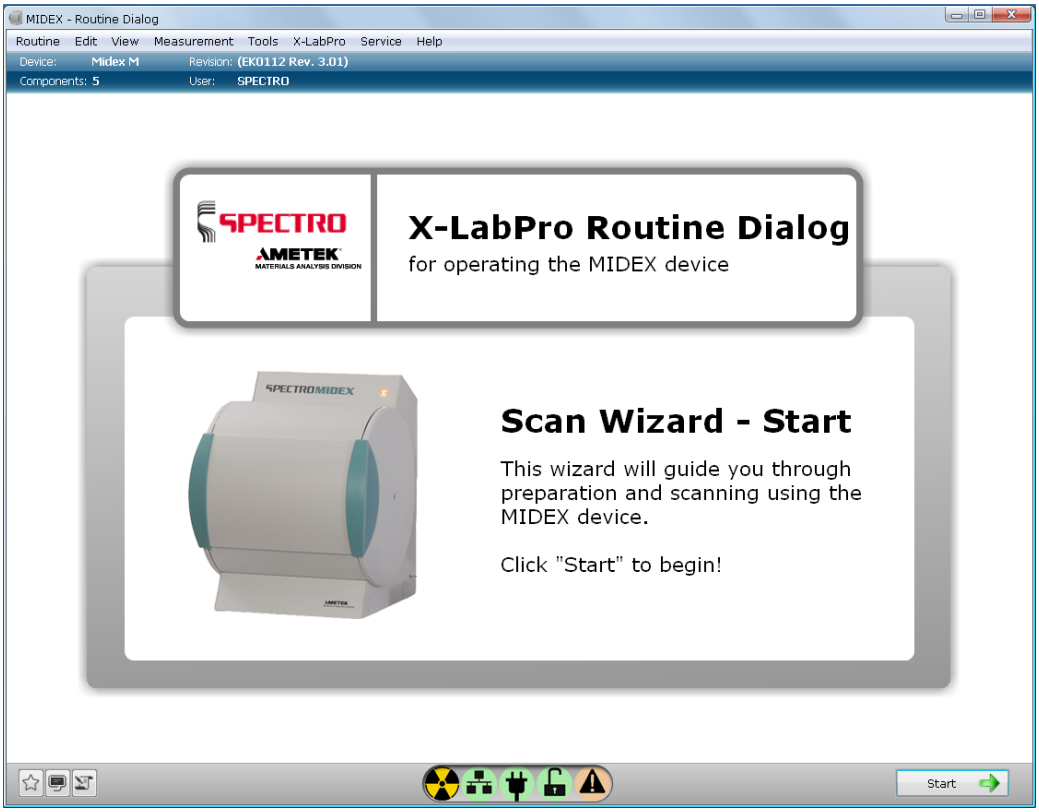
When launching the application it always shows the same state: The welcome page. This is where the process starts.

25.6.1 Wizard Workflow

Chapter 2.4 Quick Scan Gide gave a brief introduction on the workflow of the Routine Dialog. The following list shows how the wizard style Routine Dialog advances through the process of scanning a sample step by step:

ID	Page	Task
1	**Welcome Page**	Start page of the application shown after login and connecting
2	**Stage Setup Page**	Define the maximum Z position (height) of the stage/ sample, set camera properties (e.g. zoom level), define light intensity, calibration tasks
3	**Preview Scan Page**	Scan a preview image of the stage/sample. This preview will be used to define the scan positions. There are two scan modes available: Raster Scan and Point and Shoot.
4	**Scan Setup Page**	Easily navigate over the preview image and define the spots to scan using Mapping mode, Linescan mode or Pointscan mode.
5	**Verification Page**	Review your setup and select an evaluation mode (fast or advanced)
6	**Scan Progress Page**	During the scan the Scan Progress page shows intermediate results and the remaining time until the scan is finished. When finished the Page automatically switches to the next page:
7	**Scan Results Page**	Review the results of the scan using Color Maps View, Spectra View (Pointscan only) or Results List View (Pointscan only)

25.6.2 Welcome Page



The Welcome Page is shown after the application is launched and initialized. This page is meant to give an overview of the initial state of the device before entering the scan process.

Use this dialog to check if the device is connected properly (see chapter 4.2 Connecting the Device); check if the simulation mode is deactivated (unless you want it to be active) and if the device parameters are correct.

When the application initializes there may be some messages notifying about required actions. For instance if the high voltage of the X-ray generator is active at launch a message will ask to shut the voltage down.

In case of errors during the connection initialization of the application (e.g. if no device could be found) an error message is displayed. The application will exit after closing the message box.

After successful connection another message will ask if the standby mode of the device should be activated (see chapter 4.4.2.1 Entering Standby Mode for more information).

When the application initialization sequence has finished, the device was connected properly and a choice about the standby mode was made, the **Start** button of the wizard navigation gets enabled.

Click the **Start** button to begin the scan process using your MIDEX device and the MIDEX Routine Dialog. The wizard switches to the Stage Setup Page (see chapter 4.4.3)

25.6.2.1 Entering Standby Mode

When standby is activated the X-ray generator runs on a level defined in the X-Lab^{Pro} configuration editor. The shutter, protecting the sample chamber from X-rays, remains closed. It is safe to open the chamber and place a sample on the stage.

The device remains in standby until a scan is started. After the scan has finished, the standby mode will be reactivated.

	The standby mode becomes active after every scan, even if it was not activated before.

	Never switch off a device running in standby mode using the hardware switch. This could drastically reduce the lifetime of the X-ray tube or cause direct damage to it. The X-ray tube requires to be shut down softly by the MIDEX Routine Dialog to ensure a maximum lifetime

25.6.3 Instrument Setup Page

The Instrument Setup dialog is used to prepare the device, the stage and the sample for the scan setup. It is suggested to process the following task remaining their order:

Place the sample onto the center position of the stage
When the sample stage initializes it moves to the lowest possible position. This makes it easy to place the desired sample onto it. It is recommended to put it into the middle of the stage. Leave the door to the sample chamber open for now.

Move the sample to the center position of the camera live image
Use the stage navigation controls (see 4.4.3.2) to move the sample to the middle position of the live image. Use the crosshair displayed on the screen as point of reference.

Lift the stage carefully to the top of the sample chamber
This step needs to be handled very carefully! Lifting the stage too high can push the sample into the detection system and cause damage to the device. Use the stage navigation controls (see 4.4.3.2) to lift the stage to the top of the chamber **without** touching it. If your device uses 2 mm distance for measurement, be sure to have the sample at least at that distance. Move the last centimeters using the

fine adjustment buttons.

Lock the maximum stage position
After reaching the desired position click the **Lock Z Position** button. This position of the Z-axis will be written to the hardware controller of the MIDEX device. During all following steps the stage cannot be lifted higher than the locked position.

If you put another sample into the chamber the position must be defined again.

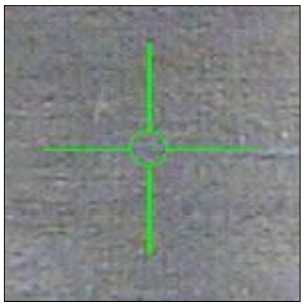
Set the camera preferences
You are free to set a camera zoom level and the intensity of the lights inside the chamber.The following image shows the Stage Setup page. The table below describes its components. For details about these controls see the following chapters starting at chapter 4.4.3.1 Live Video:

1	Live Video Image	See chapter 4.4.3.1

2	Stage Navigation Controls	See chapter 4.4.3.2
3	Camera Controls	See chapter 4.4.3.3
4	Maximum Z-Lock Switch	See chapter 4.4.3.4

25.6.3.1 Live Video

The live video control displays a realtime video image of the stage. The center of the live video displays a crosshair. This crosshair can be used as a point of orientation. The crosshair can also be used when calibrating the device or defining the right distance for measurement (see 4.4.3.4.1 Finding the right distance for measurement).



	The crosshair marks the center of the image captured by the camera. This point is not equal to the point of the X-ray beam. The offset may vary for each device and was calibrated during production.

25.6.3.1.1 Live Video Settings

The video image color settings can be dynamically adjusted. To modify these settings and save a current image of the sample stage the Routine Dialog offers a context menu on the live video control. Right click on any part of the live video to open the context menu and choose the desired option.

The color settings of the camera applied at startup are defined in the device configuration file (.xcf). The default settings can be modified using another context menu item.

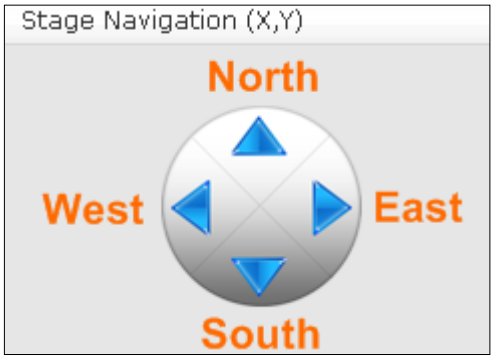
The following functions are available:

1	**Video Color Settings** – opens a dialog to modify the color options of the camera. See 4.4.3.2
2	**Reset Color Settings** – resets the color settings to default as defined in the

	configuration file.
3	**Save Color Settings to Config** – changes the default settings in the configuration file to the current settings
4	**Capture Image** – opens a Save Image Dialog Box to save a snapshot of the current camera image

25.6.3.2 Stage Control

The MIDEX Routine Dialog allows moving the sample plate into 3 directions: left/right, back/forth and up/down. The navigation left/right and back/forth can be controlled like moving over a street map using north, east, south and west directions. The MIDEX Routine Dialog offers a navigation wheel for intuitive navigation in these directions:



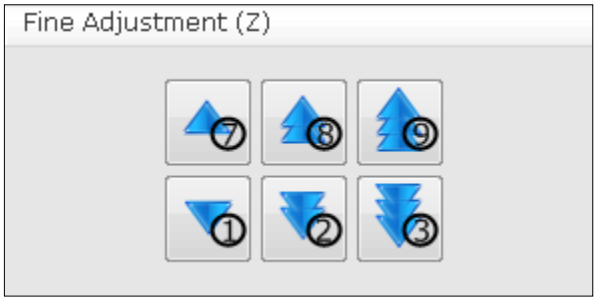
Push the button leading into the desired direction to move the stage. The button can be pushed and hold to move continuous. Leave the button to immediately stop the movement. The faster the button is hit and left, the smaller is the distance the sample stage moved.

Similar to these navigation buttons the interface provides buttons to move the sample plate up and down:

The lift and lower buttons work like the navigation wheel buttons. Holding the button moves the sample plate continuously into the corresponding direction.

These buttons should only be used as long as the distance to the detection area at the roof of the sample chamber is large enough. If the distance gets lower use the

fine adjustment buttons supporting movement of the sample plate in very small steps:



These fine adjustment buttons move the sample plate up or down like the former buttons but they behave differently. If a button is pushed the stage moves a defined length. If the button is held down, the plate does not move continuously, it moves a pre-defined amount of motorsteps. There are three different (but small) distances to move the stage. It is recommended to test the movement using the fine adjustment buttons in a safe distance to get a feeling for the distance moved.

For easier and faster handling of the stage the MIDEX Routine Dialog supports navigating by keyboard. Every navigation button of the Routine Dialog has a corresponding keyboard button:

Cursor Keys (Up/Down/Left/Right)	Navigate North, East, South and West like using the Navigation wheel
Page Up/PageDown Keys	Lift or lower the sample plate like the lift and lower buttons of the interface
Num Pad 7, 8, 9	Lift the stage in small steps like the fine adjustment lift buttons (number on the button matches the key on the number pad of the keyboard)
Num Pad 1, 2, 3	Lower the stage in small steps like the fine adjustment lower buttons (number on the button matches the key on the number pad of the keyboard)
Num Pad /	Switch the **light** on/off

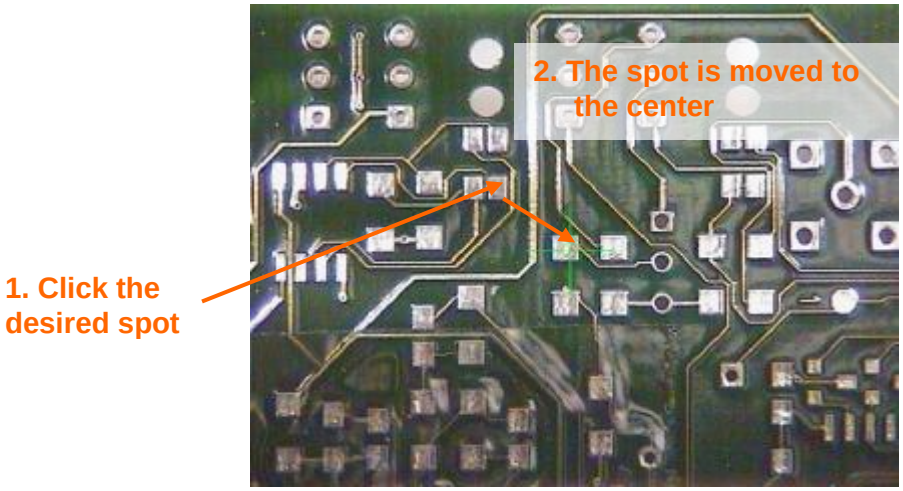
Num Pad *	Switch the **laser** on/off

25.6.3.2.1 Point and Shoot Navigation

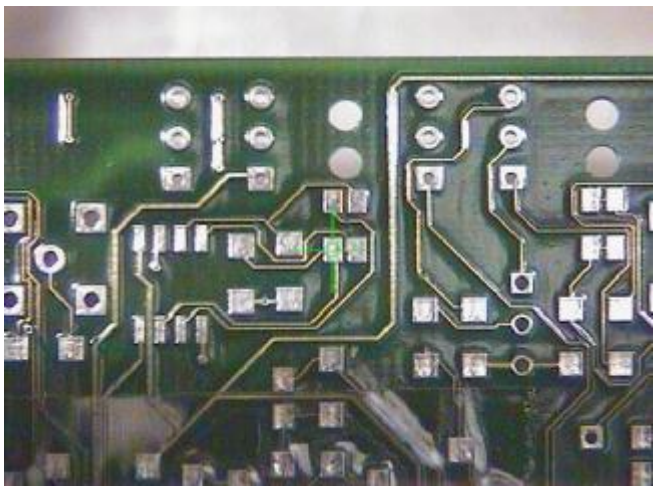
Another option to navigate north/east/south/west directions is Point and Shoot mode, named after the MIDEX Routine Dialog fast preview scan mechanism (see 4.4.4.3 Point and Shoot Scan). The functionality of this navigation option is very intuitive and fast to use. By clicking into any part of the live image, the clicked spot will be moved to the center of the crosshair.

Very easy: Left-click onto the position you whish to be the center of the live image and the stage moves it automatically to the center.

Before:

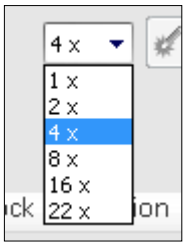


After:



25.6.3.3 Camera Control

The camera controls can be used to define the zoom level of the camera image, adjust the brightness of the light inside the sample chamber and to set the intensity of the laser.

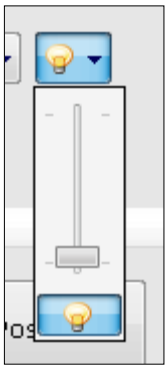


The Zoom level of the camera image can be chosen from a dropdown box provided by the stage setup page. The available zoom factors are configured in the device configuration file. The values can be edited using the X-Lab[Pro] Configuration Editor.

When selecting a different zoom level it is immediately applied to the camera.

	Zoom levels in the dropdown list are relative to the initial setting (1x) and may not be equal to the real measurements of the sample.

25.6.3.3.1 Light Level

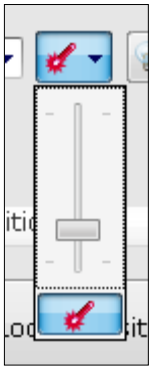


The light level (brightness) inside the sample chamber can be adjusted using the slider of the dropdown area of the light button. Clicking the other part of the button toggle the light on/off.

Move the slider to increase or decrease the brightness level until the desired result is reached. Then just click outside of the button area to close the slider.

A glowing bulb signals the light is switched on, a gray bulb shows the light is switched off. If the light is switched off and on again, the former brightness level is restored.

25.6.3.3.2 Laser Intensity



The laser intensity can be adjusted similar to the light adjustment button. Click the button to toggle the laser on/off. Open the slider and move it to increase or decrease the laser intensity.

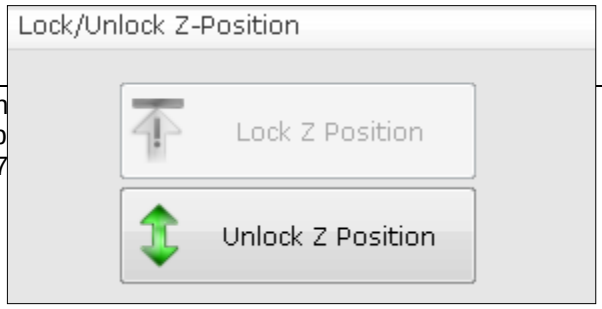
Review the state of the laser in the live video image.

	The laser is calibrated to match one defined zoom level and because of that the laser can not be used in any other defined zoom level. In this case the Laser button is disabled.

25.6.3.4 Define the Maximum Z-Position of the Stage

Defining the maximum position means also defining the measurement distance. The distance required for measurement depends on your device. Possible distances are 2mm and 20mm. As stated before, this step requires to move the sample to the center of the video image and to lift the sample plate up to the measurement (or maximum) position.

The following chapter 4.4.3.4.1 describes in detail how this position can be determined using the MIDEX Routine Dialog.



If this position is reached click the **Lock Z-Position** button to define the distance. Now the position of the Z axis is written to the device what makes it impossible to lift it higher during further processes.

If the position needs to be readjusted click the **Unlock Z-Position** button to do so. Now the movement options are available again until the **Lock Z-Position** button is clicked again.

If the maximum position was defined, the **Next** button of the wizard navigation gets active and it is possible to proceed to the next wizard page **Preview Scan**. See chapter 4.4.4 for more information on scanning a preview image.

25.6.3.4.1 Finding the right distance for measurement

The right position can be determined using the laser. The laser is configured to be exactly at the center (crosshair) position of the live video if the right distance for measurement is reached.

This setup is used to support samples of variable height. The following process is the same as described in chapter 4.4.3 but this time it includes the laser to determine the right measurement position:

1. **Place the sample to the center position of the stage**
   Move the sample to the center position of the camera live image
   Be sure to move the highest part of the sample into the center. This prevents from touching the sample chamber roof and damage the detection area.

   ⚠ **Lift the stage carefully to the top of the sample chamber**
   a. Turn the laser on and choose the optimal intensity
      (Lower intensities are better for reflecting surfaces)
   b. Lift the stage up until the sample is near the roof of the chamber.
   c. Stop movement in a safe distance before the roof.
   d. Review the live video image and step upwards using the fine adjustment buttons. Remember to take care of the distance between roof and sample.
   e. If the laser dot is exactly in the center of the crosshair the measurement position is reached. Adjust by stepping up and down until that position is reached.

2. **Lock the maximum stage position**

3. **Set the camera preferences and proceed to the next wizard page**

25.6.4 Preview Scan Page

The MIDEX Routine Dialog supports two different modes to scan a preview image: **Raster Scan** and **Point and Shoot**.

	It is recommended to close the chamber door at this point. Best preview scan results are reached using the internal illumination of the device

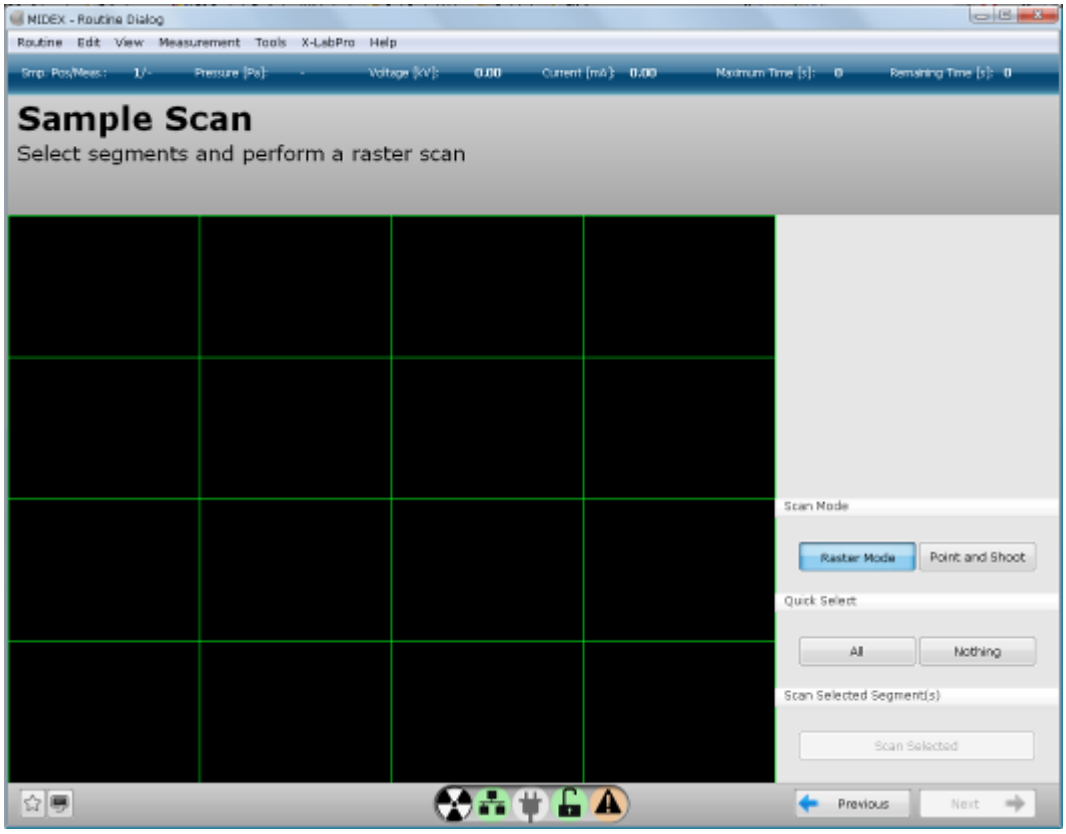
25.6.4.1 Scan Modes

Both scan modes support the creation of a preview image taken from the sample inside the sample stage. In most cases a single capture of the camera is not sufficient, for instance to create large Mappings across the sample. In this case the whole sample plate can be scanned by moving a piece of the sample plate below the camera and creating a snapshot, then moving to the next piece (or segment) and so on. All segments are combined to a big (raster) image.

Another, faster option is Point and Shoot. It supports moving the stage quickly to a desired position and capturing the segment. Then it can be directed to the next desired segment and so on. This mode is recommended for small parts of the sample to be scanned (e.g. Pointscans)

25.6.4.2 Raster Scan

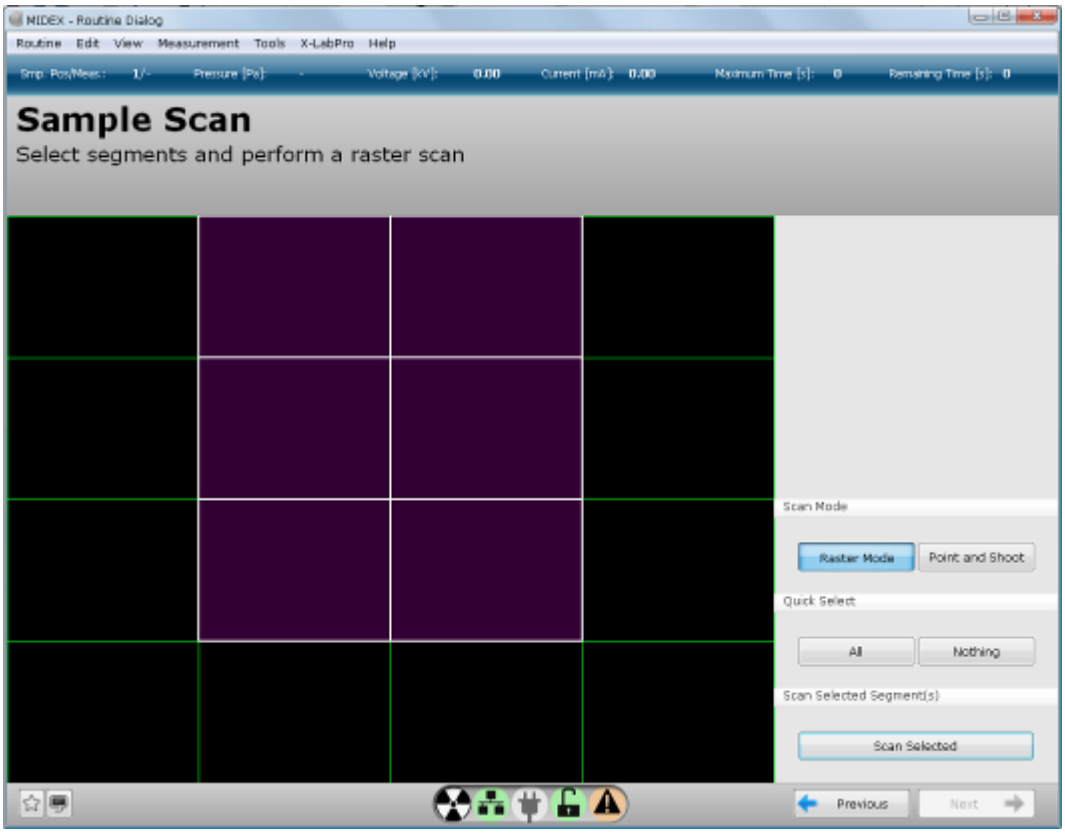
The Raster Scan page shows a representation of the stage (as black plate) separated into segments. The amount of segments is defined in the device configuration file and can be edited using the X-Lab^{Pro} Configuration Editor.



At this point there is no preview scanned and no segment selected for scanning, all segments are black. The next step is to define which segments to scan. Every combination is possible. If it is sure that a segment does not contain a part of the sample or if there is no spot to scan, the segment does not need to be selected.

To select a segment just click it. The segment changes its color. To deselect an already selected segment click it again. The segment will turn black again. To quickly select all segments click the **All** button, to deselect everything click the **None** button.

When every desired segment is selected, the selection may look like this:

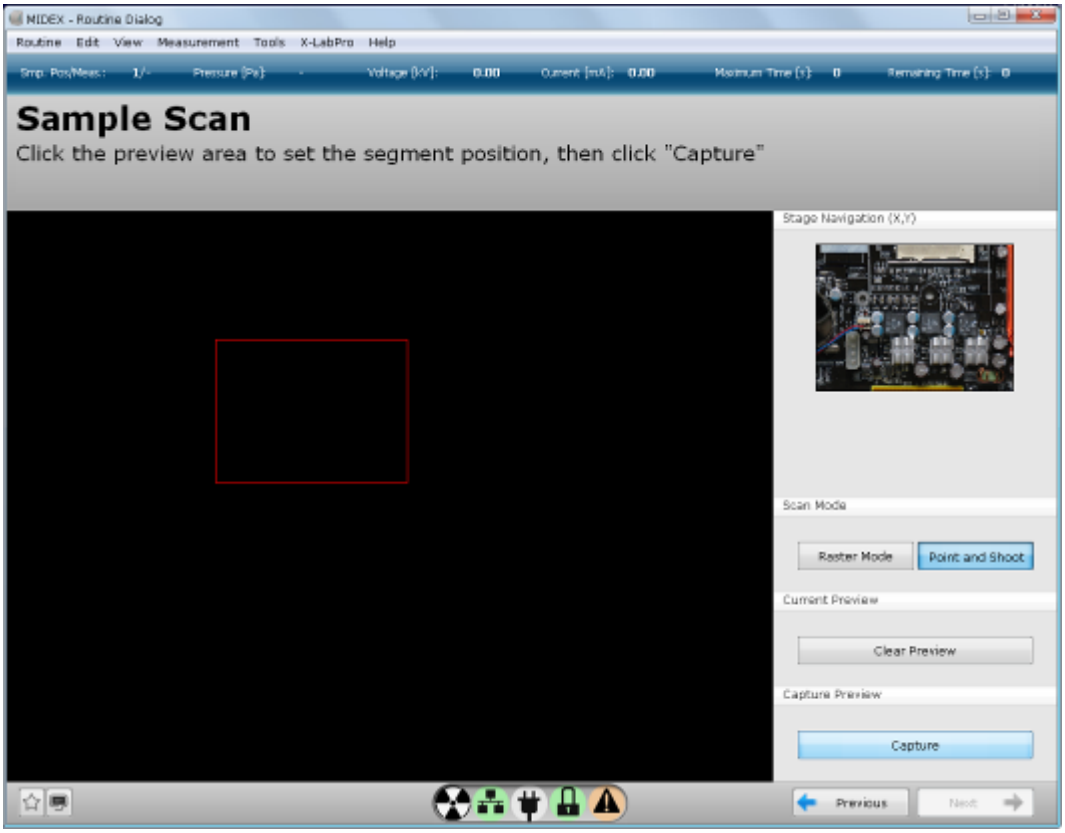


To scan the preview, click the **Scan Selected** button and wait until the scan process has finished. The MIDEX Routine Dialog application will move the sample plate and capture all segments of the sample fully automated. It is not possible to perform any tasks during this process.

If you wish to abort the operation click the **Abort Scan** button (Scan Selected has changed). The scan will stop and the partly created preview image will be deleted.

25.6.4.3 Point and Shoot Scan

The Point and Shoot Scan mode, like the Raster Scan (see previous chapter) displays a black presentation of the stage. But here the stage is not separated into segments. The Point and Shoot page displays a single segment as a red rectangle. This segment can be dynamically moved across the sample plate.



To define the exact position of the segment on the sample plate click into an area near the desired position on the black field. The stage will be moved to display the clicked spot in the center (crosshair) of the live video image on the right side of the Point and Shoot page.

You can use Point and Shoot navigation on the miniature live video image as described in chapter 4.4.3.2.2. This allows defining the position exactly. Click the part of the sample you wish to be in the center of the live video. The application will move the stage there automatically to the target position.

Verify the desired part of the sample is visible in the live video image, then click **Capture** to add this segment the preview image. Repeat these steps until all parts of the sample needed for scanning are visible.

	The best results can be received if the segments scanned do not overlap.

If the preview image fits your needs (and you have at least one segment captured), click **Next** to go to the Scan Setup Page.

25.6.5 Scan Setup Page

The Scan Setup page is the most important page of the scan setup process. This is where you can define the spots or parts of the sample to scan. You can define method and scan duration for each scan. This is what the page looks like:

1	Scan type selection tab
2	Toolbar for edit modes - Add Mode: Allows adding entries - Delete Mode: Allows removing entries - Grab Mode: Grab and move the preview image - Zoom Mode: Draw a rectangle on the preview to zoom in to the rectangle area and - Full screen: Shows the complete preview

	image inside the preview area - Options: Opens an options tool window
3	Toolbar for saving and loading list entries to/from a file.
4	**Preview area**
5	Thumbnail preview
6	Zoom selector
7	Mapping Entry – a table entry presented in the preview window
8	Information Fields – Shows coordinates of the cursor position on the preview.
9	Setup properties – Choose Method Class for scanning and define the units to show
10	Table with scan entries – one entry is one Mapping, Linescan or Pointscan. Table values (method, duration, coordinates, etc.) can be edited.

25.6.5.1 Toolbars

The scan setup page offers two different toolbars. The first is used to switch edit modes, the second offers options to save or load from/to the current table setup.

Add Mode

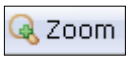
Toggles the ability to add Mappings by drawing them into the preview image.

Delete Mode

Toggles the ability to remove entries from the table

Grab mode (enabled by default)

Toggles the ability to click and hold inside the preview and drag the preview image. This moves the visible section of the preview image the amount the mouse cursor was dragged.



Zoom Mode

Toggles the ability to zoom into a smaller area of the preview image by drawing a rectangle around the desired region.

Fullscreen

Switches the zoom slider to show 100% of the scanned image inside the preview area.

Options

Opens a window to adjust the color of the Mapping presentation on the preview image and to save the preview (full stage image) as image file.

Load Table

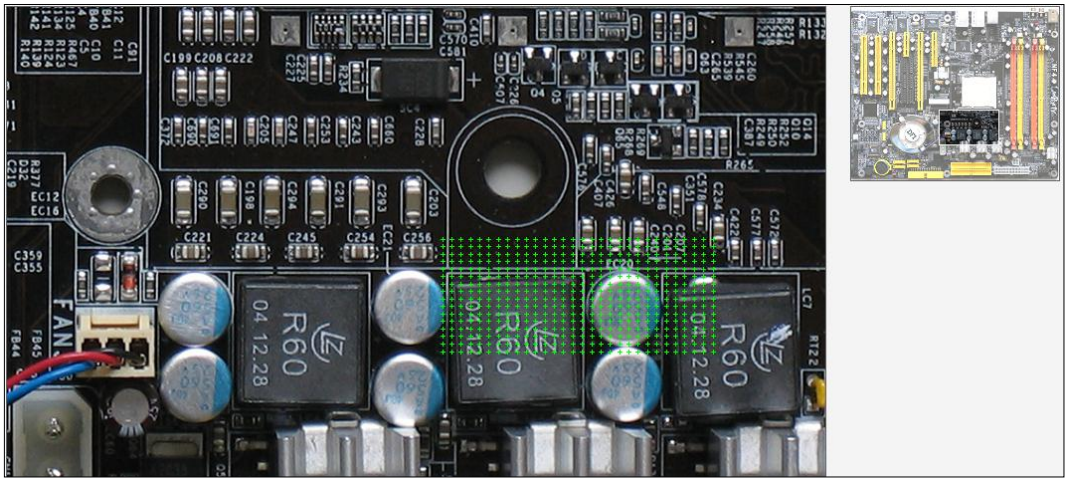
Opens a dialog box to load a previously saved list of Mapping, Linescan or Pointscan entries. (depends on scan type, see chapter 4.4.5.8)

Save Table

Opens a dialog box to save the current list of Mapping, Linescan or Pointscan (depends on scan type, see chapter 4.4.5.8) entries into a file.

25.6.5.2 Preview Image

The Preview area of the scan setup page is divided into two controls. The larger main preview is used to perform actions like adding Mappings, the smaller thumbnail preview is used to show which section of the complete image is currently visible in the main preview (see next chapter 4.4.5.2.1 for more information on the thumbnail preview).



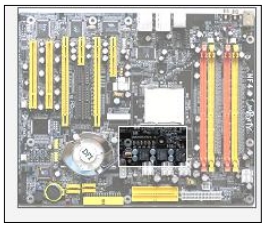
The main preview area shows the scanned image generated in the previous wizard page (Raster Scan or Point and Shoot). The zoom level and the portion of the image visible in the preview area can be defined dynamically using the zoom and navigation tools provided on the scan setup page. See chapter 4.4.5.3 for more information on zooming and chapter 4.4.5.4 for more information on moving the image to display a desired region of the preview.

If there are entries in the table, the preview shows these Mappings, Linescans or Pointscans as crosses or as lines/rectangles if the zoom level is too small to display crosses. The color of the crosses can be defined in the options tool window. Each cross represents a point to scan. See chapter 4.4.5.9 for more information on scan positions and how they are defined.

	The main preview displays only entries of the current scan mode (Mapping, Linescan, Pointscan) defined by the activated tab on top of the scan setup page (see 4.4.5.8)

	If an entry is not visible in the main preview this be caused by wrong coordinates (e.g. outside the preview), too low resolutions (0 or 1) or a mark color similar to the background of the sample (e.g. black on black).

25.6.5.2.1 Thumbnail Preview



The thumbnail preview area shows a miniature version of the full image scanned before. It marks the region of the image which is currently presented in the main preview area. The thumbnail preview can be used to navigate over the full stage preview image by dragging the section rectangle. Short clicking inside the thumbnail preview area moves the center of the section rectangle to the clicked spot. The main preview is updated immediately.

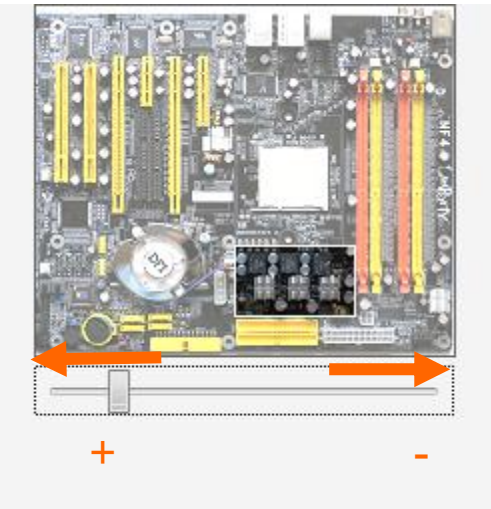
25.6.5.3 Zooming the preview

The scan setup dialog supports zooming in and out of the preview image. Using image zoom you can easily define a position on the image exactly (up to one pixel). On the other side it is easy to have an overview of the whole image or large areas of it (by zooming out).

To completely zoom out use the **Fullscreen** button of the toolbar or simply **right click** into the main preview area. The main preview updates to show the complete image scanned before. If there is a portion of the main preview area left (e.g. because of the aspect ratio) this part is filled using black color. The zoom level cannot be set lower than this.

To zoom in using the preview image there are two possibilities:

The Zoom Slider



Below the thumbnail preview area a zoom slider control is displayed. Moving the slider increases/decreases the zoom level. Moving the zoom slider to the right decreases the zoom level, the segment of the picture shown in the main preview area gets larger.

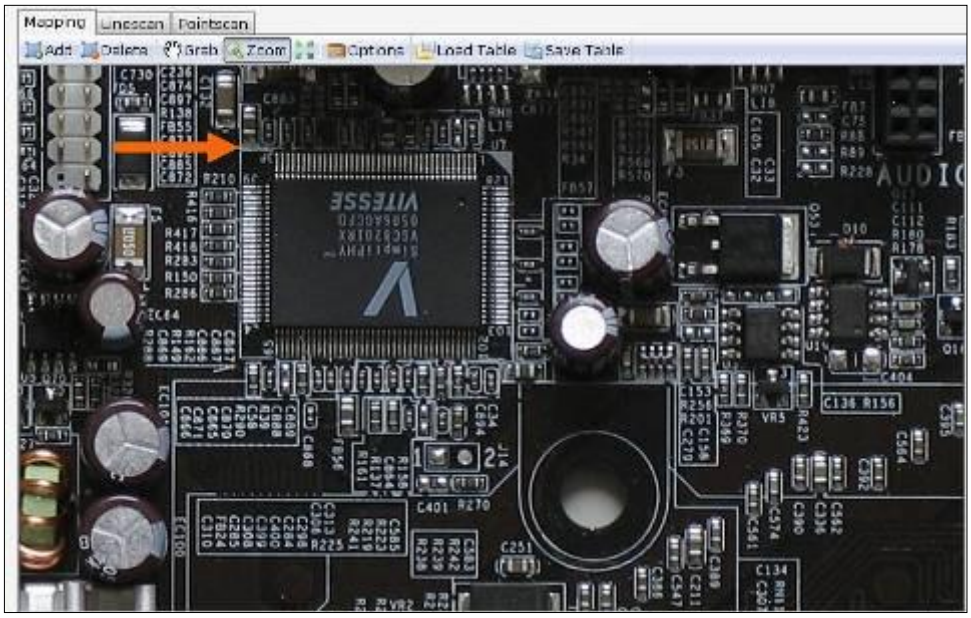
Moving the zoom slider to the left increases the zoom level, the segment of the preview displayed in the main preview area gets smaller.

The maximum Zoom level (slider fully left) is reached if the main preview area displays a segment of 5% of the full preview image.

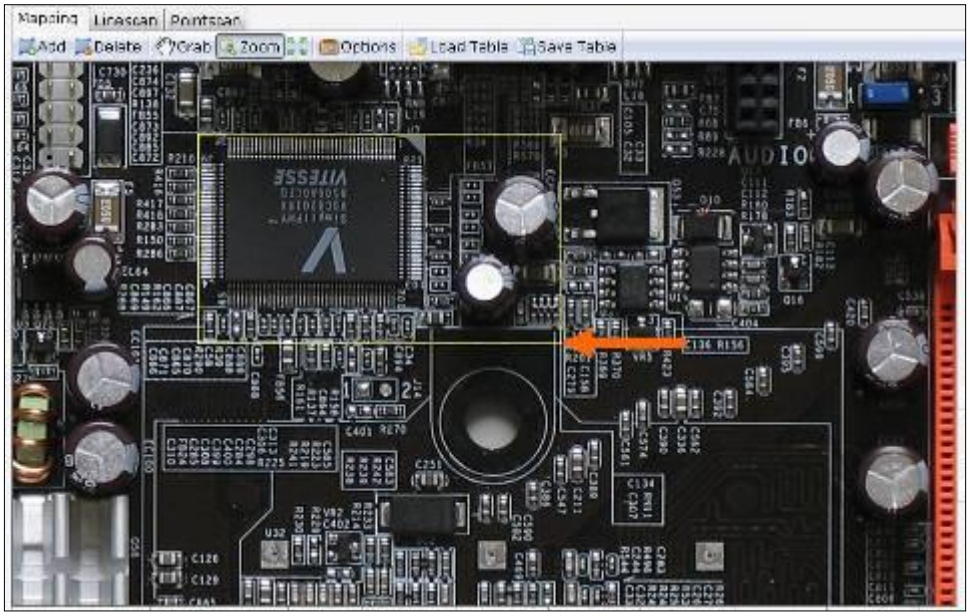
	The view will not be interpolated; upscaling increases the pixel size of the image.

1. The Zoom Mode

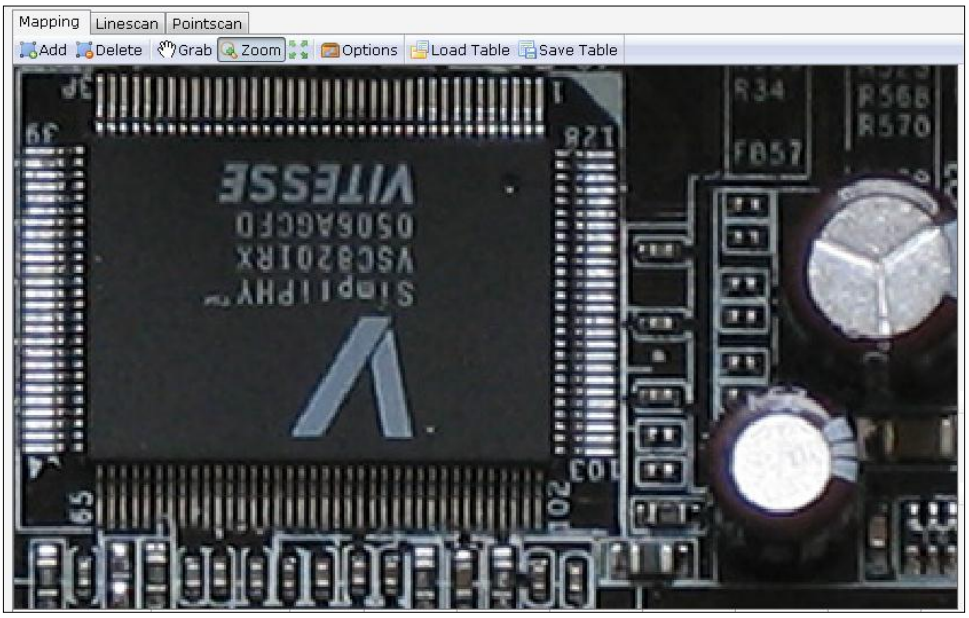
Zoom mode offers the ability to define the rectangle to be displayed directly in the main preview area. Zoom mode is activated using the toolbar button **Zoom**. Proceed as follows:



1. Click on a spot inside the main preview area as start point and hold the left mouse button down.



Drag the mouse cursor to the desired end point. Notice that the selection keeps the aspect ration automatically. Release the left mouse button to finish.



3. The main preview now shows the contents of the selection using proper scaling and moving.

Zoom mode remains active until it is deactivated or another mode was activated. It is possible to zoom in until the maximum zoom level is reached.

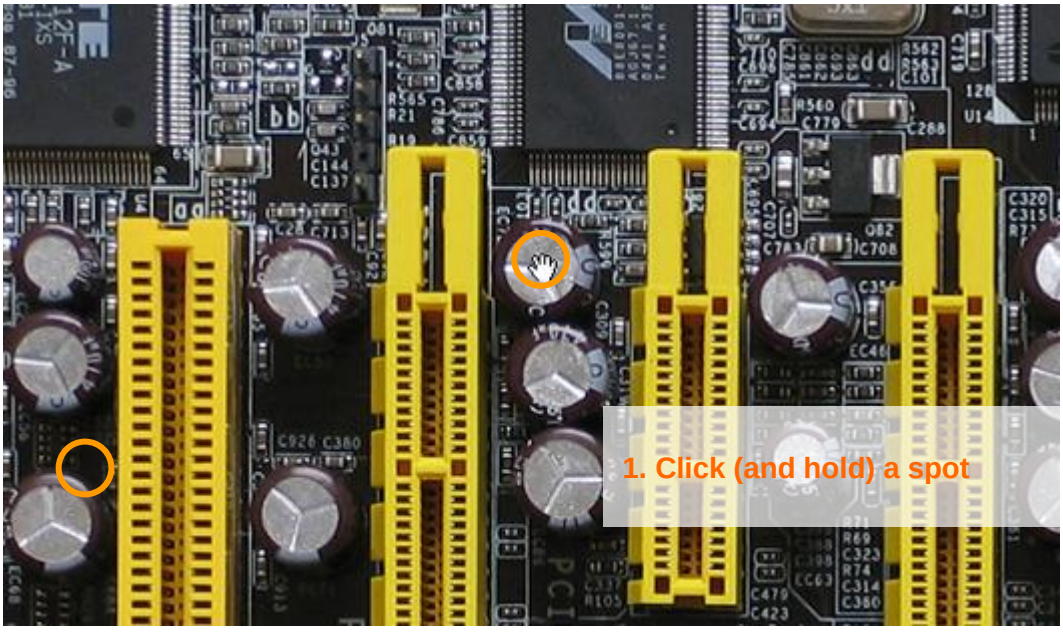
	To restart the zooming process, simply right click into the main preview. The whole image is now visible and a new region to be zoomed in to can be selected.

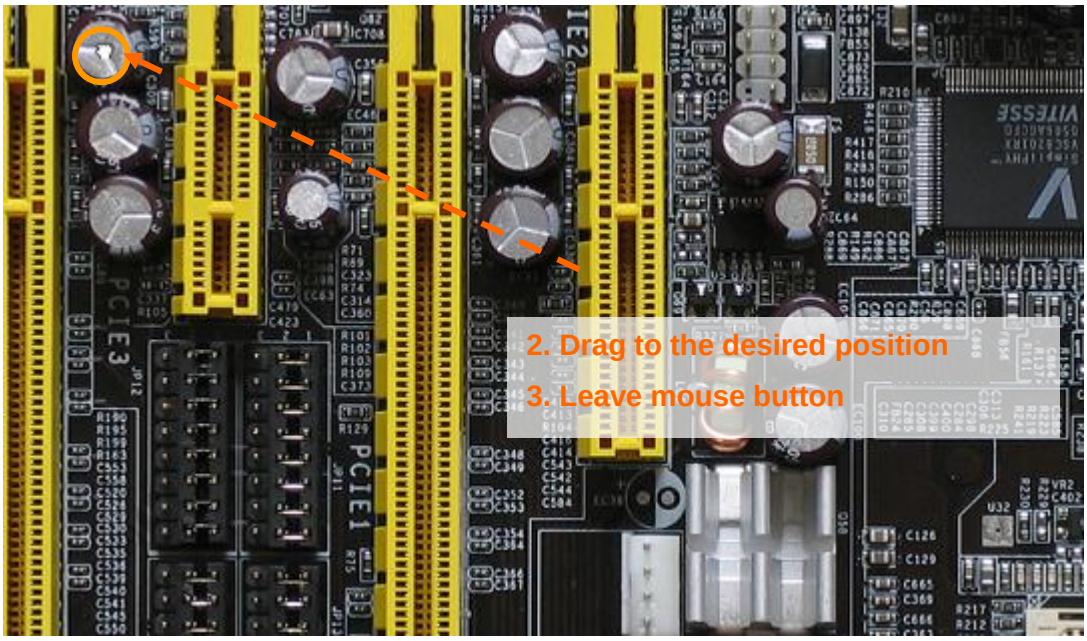
25.6.5.4 Navigating through the preview

If the zoom level is higher than the minimum, the preview image is not completely visible. During creation of Mapping, Linescan or Pointscan setups it may be necessary to move the visible area of the preview image in the preview area of the scan setup page to another position. This can be established using the grab mode or the thumbnail preview.

Grab Mode

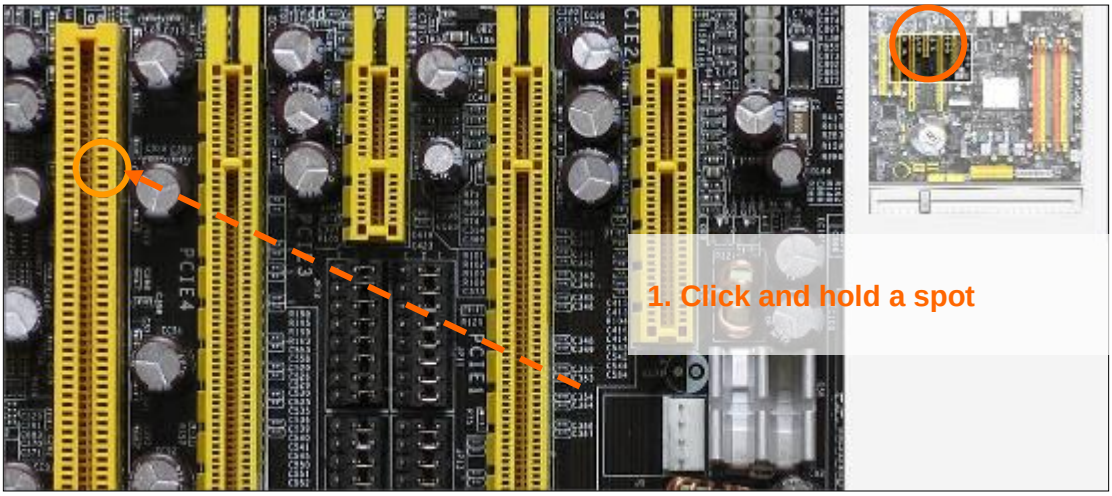
The grab mode can be used to easily move the sample preview image. It works using drag and drop. In grab mode the cursor becomes a hand when moving over the preview area. Click on any spot inside the preview area and hold the mouse button down. The hand cursor grabs the picture. Now move the mouse cursor in any desired direction, the image moves the same amount. To apply the new position just leave the left mouse button.

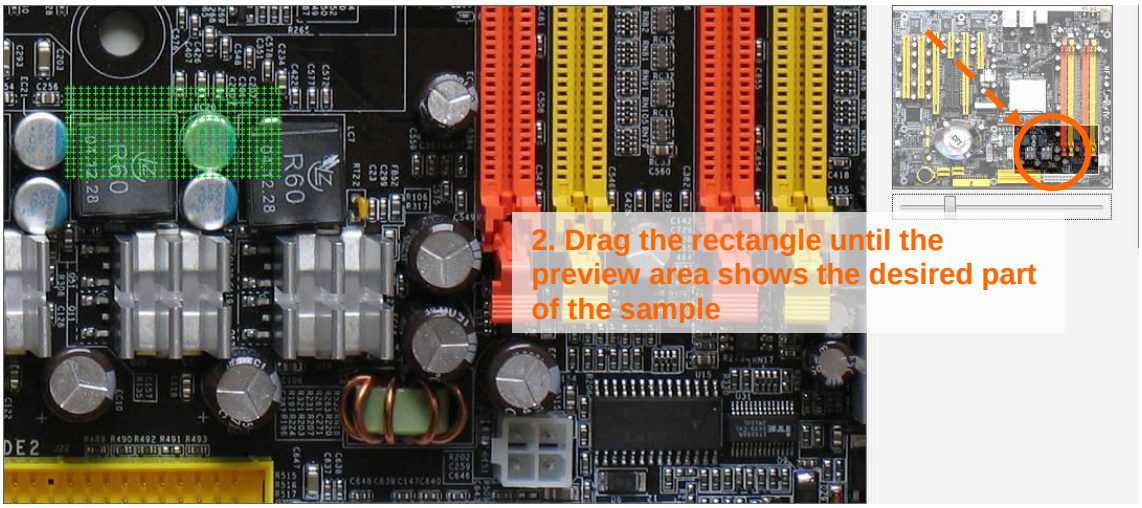




Thumbnail Preview

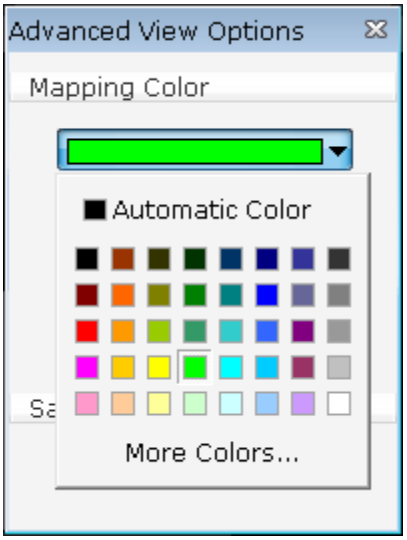
Click anywhere into the thumbnail preview image and the clicked spot will become the center of the main preview area. The zoom level will not be altered. Click, hold and drag the rectangle to review the movement and the resulting display in the preview area.





25.6.5.5 Preview Options

Click the **Options** button in the toolbar to open the **View Options** tool window. The tool window can be opened while working inside the scan setup page. It does not block input or progress on that page.

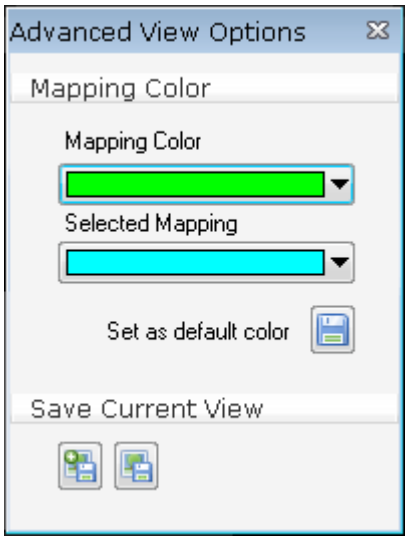


The **Mapping Color** region allows modifying the color used to mark the Mapping, Linescan or Pointscan display (crosses, lines or rectangles) in the main preview area.

The display color in the preview area will immediately change after selecting a new color. This allows checking if the color meets the requirements (high contrast to background).

Click the color drop down button to choose a different color. Choose one from the predefined set or define a new color by clicking the **More Colors** button.

The default button color is restored, if the application is restarted. If you wish to define a new default color select it and click the **Set as default color** button. This action will write the color value into the configuration file and restore it after each restart.



The Save Current View region offers possibilities to save the preview image (the complete image, not just the preview area) into a file. There are two options:

Saves the image including the presentations of Mappings, Linescans or Pointscans.

Saves the original image (without marks).

After clicking a button a Save Image File dialog box appears offering to save the image as jpg, gif, png and bmp.

25.6.5.6 Method Class and Method Selection

It is recommended to choose a method class before adding Mappings.

Method classes can be configured in the X-Lab^{Pro} Configuration Editor. By defining method classes and assigning methods to it.

	A Method class is a container for multiple methods of a similar type or for a similar purpose.

Choose a method class from the list of available method classes. The method list that can be selected for an entry in the tables will be replaced with the method list of the newly selected method class. If there are already entries in any table, a warning will be displayed. If a new method class is selected the method selection of all entries is reset to the first item of the new list.

For proceeding confirm the message, otherwise cancel it. After canceling the method class will be set back to the former setting. The table entries will not be changed.

	The method lists for Mappings and Linescans contain only those methods marked as Mapping compatible in the method administration of X-Lab^{Pro}

25.6.5.6.1 Scan Duration

When a method is selected from a dropdown item in the table (see chapter 4.4.5.9), the scan duration is automatically set to the value defined in the respective method. This default value can be edited using the method administration of X-Lab^{Pro}. The value displayed in the table can be modified and applies only to the corresponding item. If the method selection changes, the value will be reset to the value configured in the method.

	The scan duration will also be reset if a new method class was selected and the method has changed.

25.6.5.7 Saving and Loading Setup Lists

To load a scan setup file activate the tab for the corresponding scan type, Mapping, Linescan or Pointscan). Click the **Load Table** button in the Load/Save

toolbar. An Open File Dialog Box pops up requesting to choose a setup file. Choose a compatible file from your file system. The following list shows the file formats available for import:

***. mml**	**MIDEX**apping **L**ist – contains a list of Mappings
***.mll**	**M**idex **L**inescan **L**ist – contains a list of Linescans
***.mpl**	**M**idex **P**ointscan **L**ist – contains a list of Pointscans.

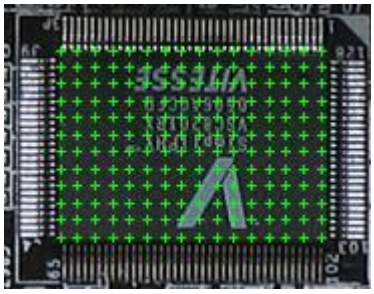
After selecting a file the list entries inside will be read and imported into the table for the corresponding scan type.

⚠	**If a file is loaded all existing table entries will be replaced by the imported entries.**

To save the list has to contain at least one item. Select the tab page for the corresponding scan type (Mapping, Linescan or Pointscan) and click the **Save Table** button. A File Save Dialog Box appears and offers to save the file as the format matching the currently selected scan type.

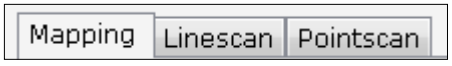
25.6.5.8 Switching Scan Types (Mapping, Linescan or Pointscan)

The scan setup page of the MIDEX Routine Dialog offers three different scan types:

Mapping	 **Management as Mapping file**	**Rectangular area on the sample** **Configurable resolution, max. 128x128 (amount of scan points horizontal and vertical evenly distributed over the area)** **Short scan duration for each point** **Simple evaluation mode only (see 4.4.6.3)** **Result view as color maps, threshold maps or threshold mix**
Linescan		**Line on the sample defined by start and end point** **Configurable resolution, max 128 (amount of scan points evenly distributed along the line)** **Short scan duration for each point** **Simple evaluation mode only (see 4.4.6.3)** **Result view as graph (XY-chart)** **Management as Linescan file**

Pointscan		**Single Point on the sample** **Longer scan duration than Mapping and Linescan** **Advanced evaluation mode** **Result view as spectrum or element listing** **Management using Job Manager of X-Lab[Pro]**

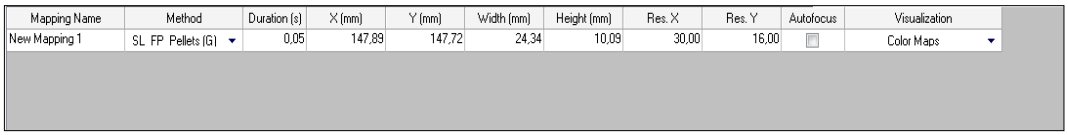
Select the scan type using the tab control at the top of the scan setup page.



Activate the desired tab to switch the view of the scan setup page to the corresponding table. The table columns differ for every scan type. The following chapter describes how the setup of a scan entry can be done.

25.6.5.9 Setup Mappings

If the Mapping scan type is activated the scan setup page shows the table for Mapping scan entries.



The following list describes the columns of the table and their properties:

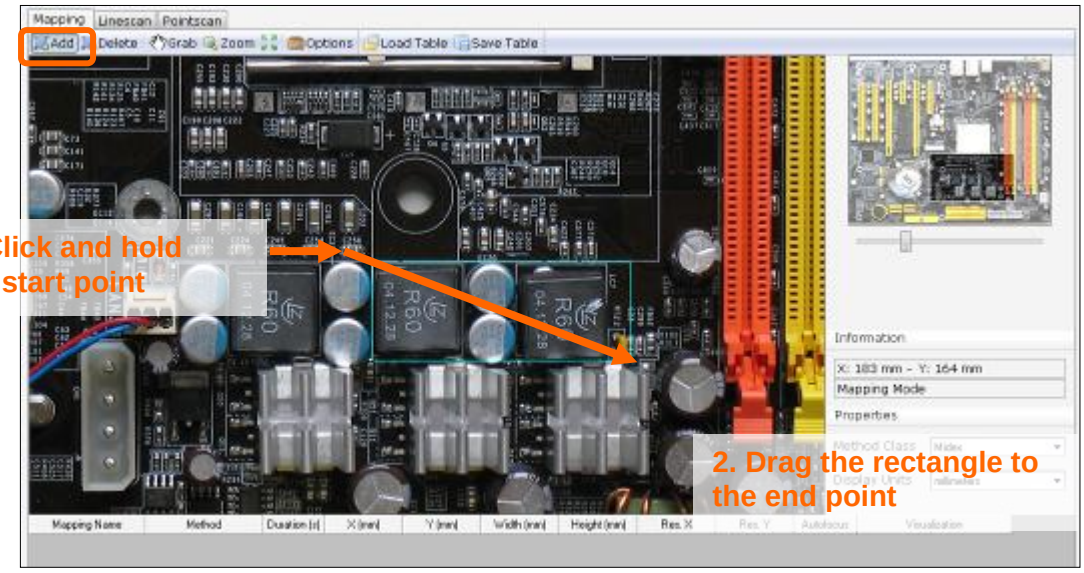
Mapping Name	Text value	A name for the Mapping entry, unique in this list. If a new Mapping is created, the application assigns a default name which can be edited afterwards.
Method	Drop down list	List of methods according to the currently selected method class (see 4.4.5.6) changing the method causes a reload of the duration cell and recalculation of the resolution.
Duration	Numeric value	Duration for scanning one point (usually millseconds for Mappings and Linescans, seconds for Pointscans).

X	Numeric value	X coordinate of the start point (units here and below as selected, see 4.4.5.12).
Y	Numeric value	Y coordinate of the start point.
Width	Numeric value	Width of the Mapping (base value to distribute horizontal scan points).
Height	Numeric Value	Height of the Mapping (base value to distribute vertical scan points).
Res. X	Numeric value < 128	Count of scan points to distribute along the width of the Mapping.
Res. Y	Numeric value < 128	Count of scan points to distribute along the height of the Mapping.
Autofocus	Checkbox	Checked to do a Z axis auto correction before each scan point (automatic adjustment of measurement distance).
Visualization	Drop down list	Selector to choose which visualization to show during scan progress.

25.6.5.9.1 Adding, Deleting and Modifying Mappings

To add a Mapping first make sure the **Mapping** tab is activated at the top of the scan setup page. Next use the zoom and navigation tools of the scan setup page to set up the preview area. Ensure the complete area required for the Mapping is visible. Then enter **Add Mode** by clicking the **Add** button of the toolbar.

In add mode click the first point of the Mapping (top left corner) inside the preview area and drag a rectangle until the desired area of the Mapping is enclosed exactly. Then leave the mouse button.



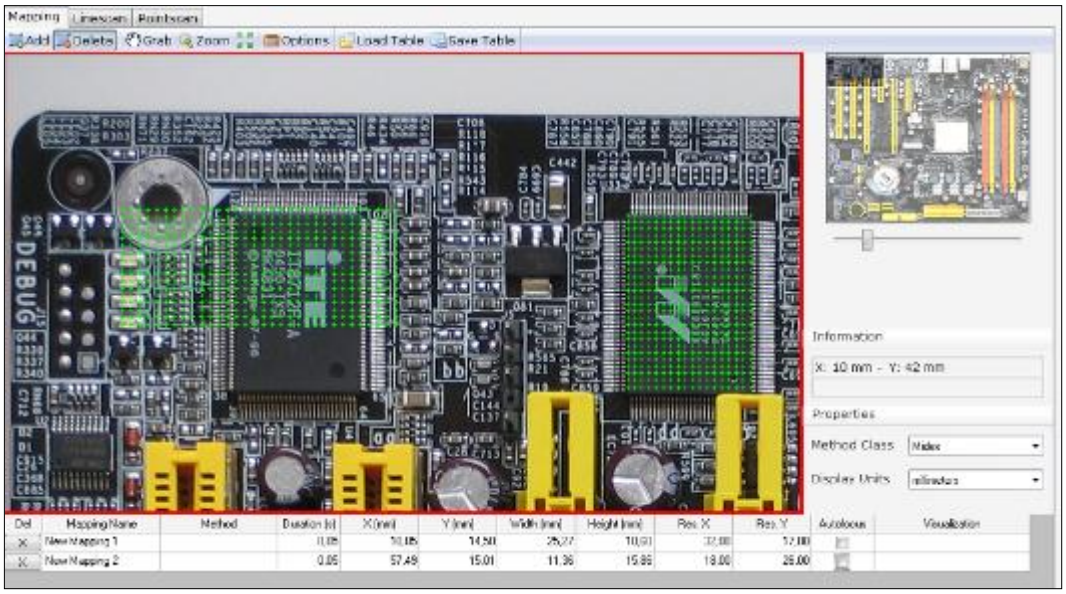
The Mapping is now added to the table at the bottom and displayed in the preview area. If the position of the Mapping is not correct and needs to be modified, this

can be done using the values in the table. Adjust a coordinate value and the change will immediately be applied to the preview. If the positioning is done choose a method from the method list in the new row of the Mapping table.

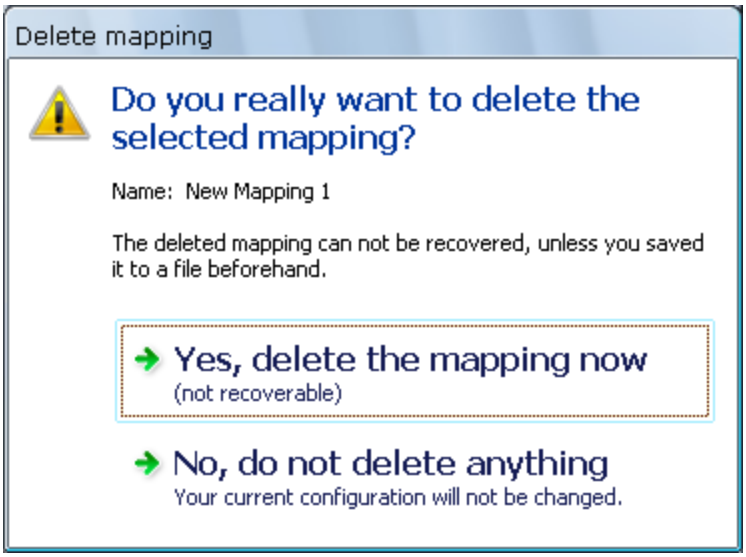
Changing the method will load the default duration for one scan point from the method data and change the duration cell of the new row. The resolution values will also be calculated after a change of the method. This calculation is based on the size of the collimator. The application calculates how many points fit into the width of the Mapping. After the method was defined, the values for duration and resolution can be edited as required.

	It is recommended to only lower the values for the resolution because a higher resolution could lead to unexpected results due to overlapping scan points.

Deleting Mappings is done using delete mode. First make sure the Mapping tab is activated and there are Mappings defined you wish to delete. Next enter **Delete Mode** by clicking the **Delete** button in the toolbar.



The border of the preview area turns red to warn that you have entered delete mode. It is important to be aware delete mode is activated to not accidentally delete a Mapping. A new column is added at the beginning of the table containing a button **X**. This is the delete button. To delete a Mapping in delete mode click on the delete button of the corresponding table ro

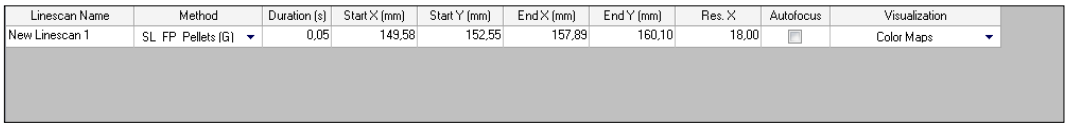

Delete mapping
Do you really want to delete the selected mapping?
Name: New Mapping 1
The deleted mapping can not be recovered, unless you saved it to a file beforehand.
Yes, delete the mapping now
(not recoverable)
No, do not delete anything
Your current configuration will not be changed.

A message box is displayed requesting to confirm the deletion of the Mapping. Click **Yes** to do so or **No** to cancel.

If you click **Yes**, the Mapping is removed from the list. The delete mode remains active after a Mapping was deleted. If the last Mapping was deleted and the table is empty, delete mode is deactivated automatically.

25.6.5.10 Setup Linescans

If the Linescan type is activated the scan setup page shows the table for Linescan scan entries.



The following list describes the columns of the table and their properties:

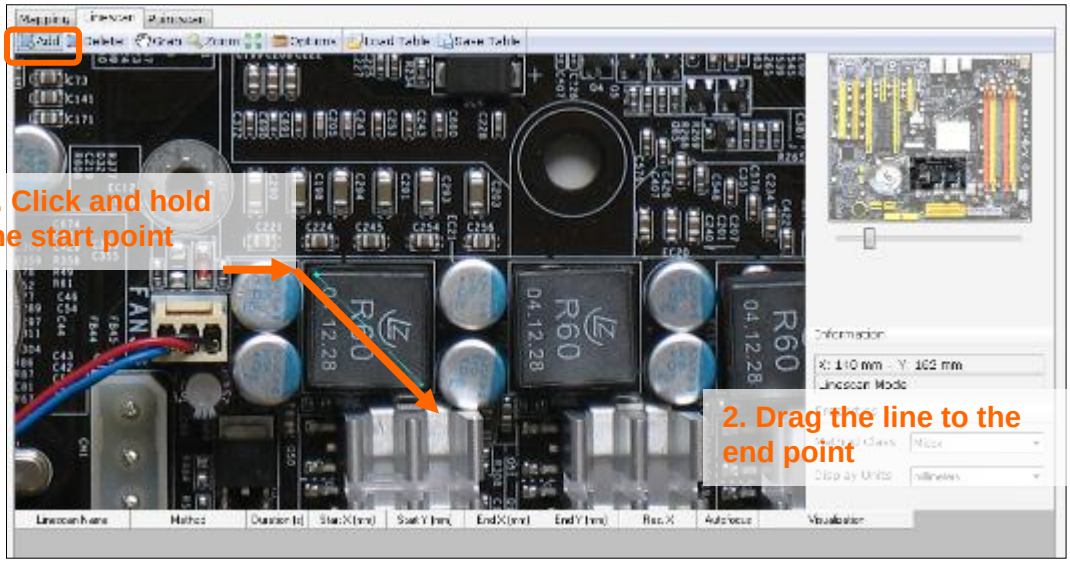
Linescan Name	Text value	A name for the Linescan entry, unique in this list. If a new Linescan is created, the application assigns a default name which can be edited afterwards.
Method	Drop down list	List of methods according to the currently selected method class (see 4.4.5.6) Changing the method causes a reload of the duration cell and recalculation of the resolution.

Duration	Numeric value	Duration for scanning one point (usually millseconds for Mappings and Linescans, seconds for Pointscans).
StartX	Numeric value	X coordinate of the start point (units here and below as selected, see 4.4.5.12).
StarttY	Numeric value	Y coordinate of the start point.
EndX	Numeric value	X coordinate of the end point.
EndY	Numeric Value	Y coordinate of the end point.
Res. X	Numeric value < 128	Count of scan points to distribute along the line defined by the start and end coordinates.
Autofocus	Checkbox	Checked to do a Z-Axis auto correction before each scan point (automatic adjustment of measurement distance).
Visualization	Drop down list	Selector to choose which visualization to show during scan progress.

25.6.5.10.1 Adding, Deleting and Modifying Linescans

To add a Linescan first make sure the **Linescan** tab is activated at the top of the scan setup page. Next use the zoom and navigation tools of the scan setup page to set up the preview area. Ensure the complete area required for the Linescan is visible. Then enter **Add mode** by clicking the **Add** button of the toolbar.

In add mode click the first point of the Linescan inside the preview area and drag a line until the desired end point of the Linescan is reached. Then leave the mouse button.



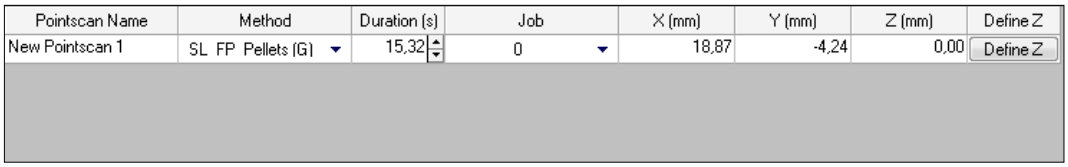
The Linescan is now added to the table at the bottom and displayed in the preview area. If the position of the Linescan is not correct and needs to be modified, this can be done using the values in the table. Adjust a coordinate value and the change will immediately be applied to the preview. If the positioning is done choose a method from the method list in the new row of the Linescan table.

Changing the method will load the default duration for one scan point from the method data and change the duration cell of the new row. The resolution value will also be calculated after a change of the method. This calculation is based on the size of the collimator. The application calculates how many points fit into the length of the Linescan. After the method was defined, the values for duration and resolution can be edited as required.

Deleting Linescans works similar to deleting Mappings, see chapter “Adding, Deleting and Modifying Mappings” for more information on deleting table entries using delete mode.

25.6.5.11 Setup Pointscans

If the Pointscan scan type is activated the table at the bottom of the scan setup page shows the table for Pointscan entries.



The following list describes the columns of the table and their properties:

Pointscan Name	Text value	A name for the Pointscan entry, unique in this list. If a new Pointscan is created, the application assigns a default name which can be edited afterwards.
Method	Drop down list	List of methods according to the currently selected method class (see 4.4.5.6) changing the method causes a reload of the duration cell and recalculation of the resolution.
Duration	Numeric value	Duration for scanning one point (usually millseconds for Mappings and Linescans, seconds for Pointscans).
Job	Drop down list extendable	The Job the Pointscan will be added to (see 4.4.5.11.4).
X	Numeric value	X coordinate of the scan point (units here and below as selected, see 4.4.5.12).
Y	Numeric value	Y coordinate of the scan point.
Z	Numeric value	Z coordinate of the scan point.
Define Z	Button	Opens a window to define the Z-coordinate for the selected Pointscan.

25.6.5.11.1 Adding, Deleting and Modifying Pointscans

To add a Pointscan first make sure the **Pointscan** tab is activated at the top of the scan setup page. Next use the zoom and navigation tools of the scan setup page to set up the preview area. Ensure the spot required for the Pointscan is visible. Then enter **Add mode** by clicking the **Add** button of the toolbar.

In add mode click the point inside the preview area to set the coordinate for scanning. To exactly adjust the point, click and hold the mouse button inside the preview area and drag the point to the right position. Then leave the mouse button.

The Pointscan is now added to the table at the bottom and displayed in the preview area. If the position of the Pointscan is not correct and needs to be modified, this can be done using the values in the table. Adjust any coordinate value and the change will immediately be applied to the preview. If the positioning is done choose a method from the method list in the new row of the Pointscan table.

Changing the method will load the default duration for one scan point from the method data and change the duration cell of the new row. The resolution value will also be calculated after a change of the method. This calculation is based on the size of the collimator. The application calculates how many points fit into the length of the Pointscan. After the method was defined, the values for duration and resolution can be edited as required.

Deleting Pointscans works similar to deleting Mappings, see chapter 4.4.5.9.1 for more information on deleting table entries using delete mode.

25.6.5.11.2 Defining The Z-Coordinate for one Pointscan

To specify a different Z-coordinate for each Pointscan in the table, the Table entry contains a **Define Z** Button. The default Z-coordinate is equal to the maximum Z-Position. The maximum Z position is also the highest position to define for any Pointscan. The lowest position is the 0 position of the Z-stage.

To define the Z-coordinate click the Define Z button in the corresponding row of the pointscan table. A tool window opens showing a live video image of the sample stage. The window allows moving the stage in Z-direction and to define camera option like it was already possible in the Instrument Setup Page.

The position defined by the corresponding pointscan row is automatically moved to the center of the crosshair. Use the laser and the Z-adjustment controls to specify the desired distance for measurement.

If the laser spot exactly hits the center of the crosshair click apply to save the Z-coordinate. This value will be set as Z-coordinate for the pointscan after the tool window was closed.

25.6.5.11.3 Pasting Pointscans from Standards

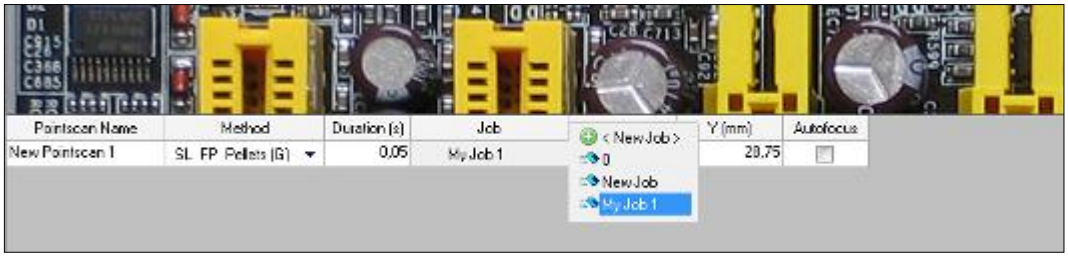
To scan standards defined in a method use the copy and paste feature of X-LabPro. The following procedure describes how to copy standards from a method and paste them into the Pointscan list:

1. Start the X-Lab[Pro] Method Administration
2. Open the desired method and choose the **Standards** tab.
3. Select the standards to scan by highlighting them in the list (use shift+click or ctrl+click to select multiple entries)
4. Right click any selected standard and select copy from the context menu. (alternatively choose Edit->Copy from the main menu or push Ctrl+C)
5. Open the MIDEX Routine Dialog, follow the instructions to perform the instrument setup and the sample scan and proceed to the Pointscan setup.
6. Add Pointscans to the list maintaining the order from the standards list in the Method Administration.
7. Mark the first list item by clicking in the name field. Standards will be pasted starting from the selected list item. This allows scanning standards and default samples from one list.
8. Choose Edit ->Paste Standards from the main menu
9. The standards are pasted to the list. All values except the coordinates are write-protected for standards. The coordinates can be changed to redefine the position of the sample on the stage.

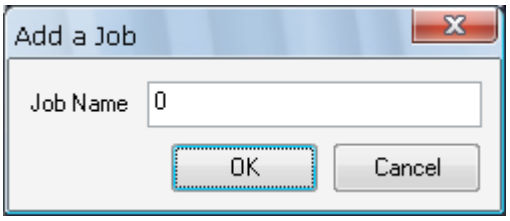
25.6.5.11.4 About Jobs

A job is a collection of scans (one or more). Jobs can be managed using the X-Lab[Pro] Job Manager. Please consult the online help of the Job Manager for more information on managing jobs.

To select a job for a Pointscan entry use the dropdown control in the **Jobs** column. By default the selection is set using a default naming pattern configurable in X-Lab[Pro] Configuration Editor (e.g. current date, week of the year, etc). This pattern is applied to the first Pointscan entry in the list. Every following item will have the job selection of its predecessor as default setting.



To change the job select another list item from the drop down list or add a new Job name by selecting the first list item **< New Job >**.

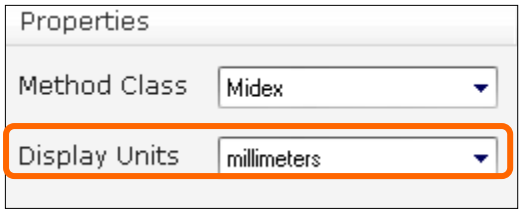


After choosing to add a new job a window opens requesting to enter a name for the new job. Enter a job name and click **OK**. The job name will be added to the dropdown list and selected for the current Pointscan.

The job name will only be assigned to the scan; it is not created in the Job Manager. The job will be created when the first item using that job name is scanned.

25.6.5.12 Stage Coordinates and Units

The MIDEX Routine Dialog allows using different units to display and configure stage coordinates. The used units can be switched using the drop down list **Display Units** on the right side of the scan setup page.



The coordinate values used in files and background processes are always handled as absolute amount motorsteps of the XYZ-stage motors starting at the initialization position of each motor.

The MIDEX Routine Dialog uses a different coordinate interpretation. Values displayed in the Mapping, Linescan and Pointscan tables are defined as distance to the top left corner of the stage (which is identical to the top left corner of the displayed preview image.

	All coordinate values displayed in the MIDEX Routine Dialog base on the top left corner of the stage (preview image)

25.6.5.13 Repro Scans

To perform repro scans first activate the **Allow Repro** setting in the Configuration Editor of X-Lab^{Pro}. This setting can be fount in the MIDEX Settings Dialog.

With repro scans enabled the pointscan tab of the scan setup page displays a dropdown field to choose a number from **1 – 20**. If **1** is selected the list is scanned only once (default mode). The selections from **2 – 20** define the number of times

the scan list will be processed. Selecting 5 means every pointscan in the list will be scanned 5 times. The Scan Verification page will display the full list including all repetitions. The routine dialog allows repeating a maximum of 10 pointscans up to 20 times.

25.6.5.14 Recalibration

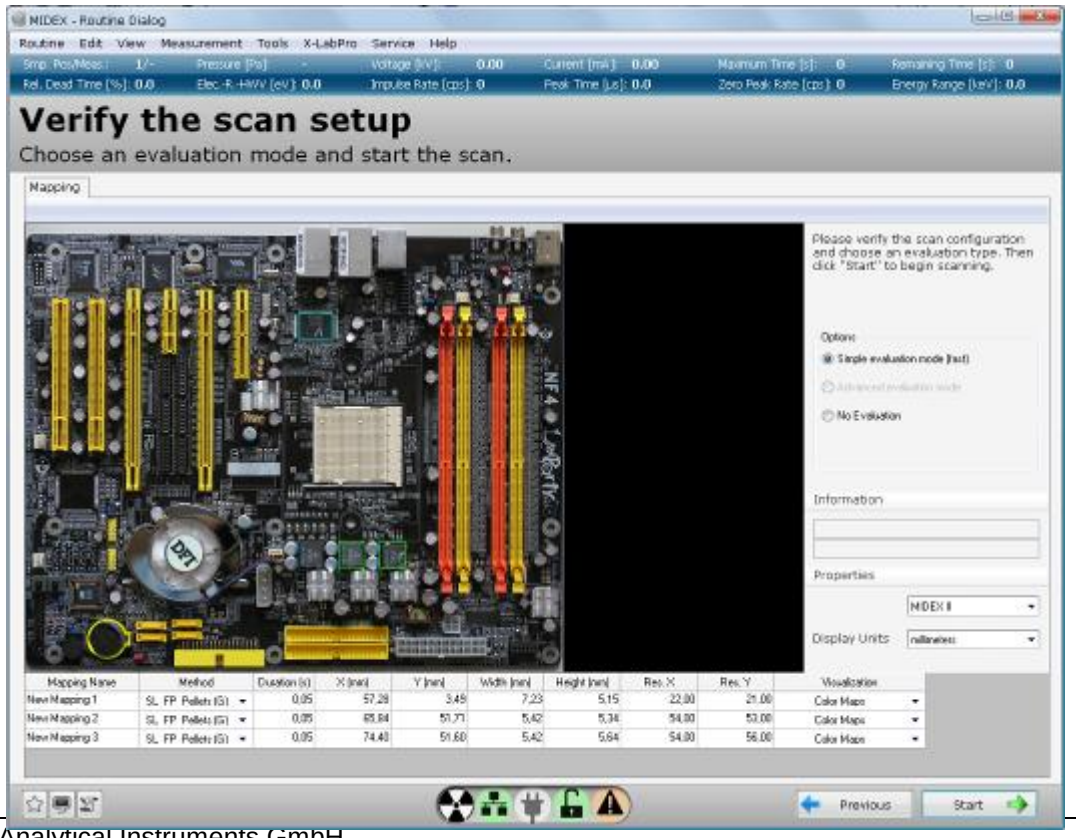
The MIDEX Routine Dialog allows recalibration using **Global** or **MCA**. To define a recalibration use the pointscan tab of the Scan Setup page. Add the appropriate number of pointscans and place them on the standards on the stage.

Choose Edit->Recalibration->Global or Edit->Recalibration->MCA in the main menu. The Routine Dialog will switch to recalibration mode. Continue the recalibration lie a usual scan.

To reset the Routine Dialog to default scan mode use Edit->Reset Table in the main menu.

25.6.6 Verification Page

After all Mappings, Linescans or Pointscans and the scan details (method, duration, etc.) are set up in the scan setup page, set the desired scan mode for the following scan. This can be done by selecting the tab on top of the scan setup page. Then click **Next** to proceed to the Scan Verification Page.

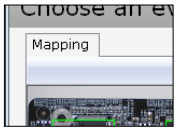

MIDEX - Routine Dialog
Routine Edit View Measurement Tools X-LabPro Service Help
Verify the scan setup
Choose an evaluation mode and start the scan.
Mapping
Please verify the scan configuration and choose an evaluation type. Then click "Start" to begin scanning.
Options
Information
Properties
Display Units
Previous
Start

The Scan Verification Page displays the selected scan mode and the setup created before. On the right side it displays evaluation options.

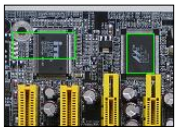
	Notice that the **Next** button of the wizard navigation changed to **Start**. This means finishing the tasks on this page and advancing in the process will finally start the measurement of the selected spots.

25.6.6.1 Review the Scan Setup

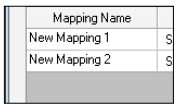
The preview area of the verification page shows the full preview image including the defined Mappings, Linescans or Pointscans. Review your scan setup as follows:



Make sure the desired scan type is selected. This is the only tab left at top of the page. If it does not match go back to the previous page, activate the desired tab and click **Next** to return to the scan verification page.



Visually check the preview image and ensure the Mappings, Linescans and Pointscans are at the right positions

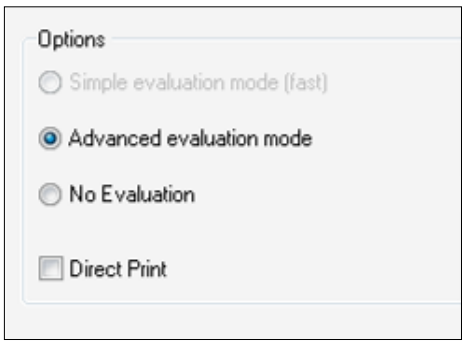


- Check the contents of the table:
  - Names correct?
  - Correct methods selected?
    - Coordinates matching desired positions?

- Right Job(s) selected (Pointscan only)?
- Visualization set correct?

25.6.6.2 Select an Evaluation Mode

On the right side of the scan verification page select an evaluation mode:



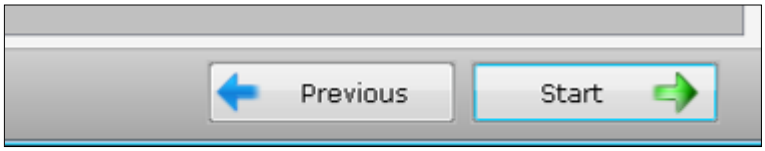
Simple evaluation mode	Only available for Mappings and Linescans. Performs a quick evaluation of the detector information without using advances evaluation algorithms. The results will be displayed as relative intensities only.
Advanced evaluation mode	Only available for Pointscans. Performs a slow but very reliable evaluation using advanced algorithms. The results will be displayed in concentration values.
No evaluation	Saves the detector information and does not run any evaluation.

The **Direct Print** option is available for Pointscans only. If this option is checked, the results are sent to the printer after a measurement has finished.

After choosing an evaluation mode and selecting the Direct Print option (if desired) everything is set up for measurement.

25.6.6.3 Start the Scan

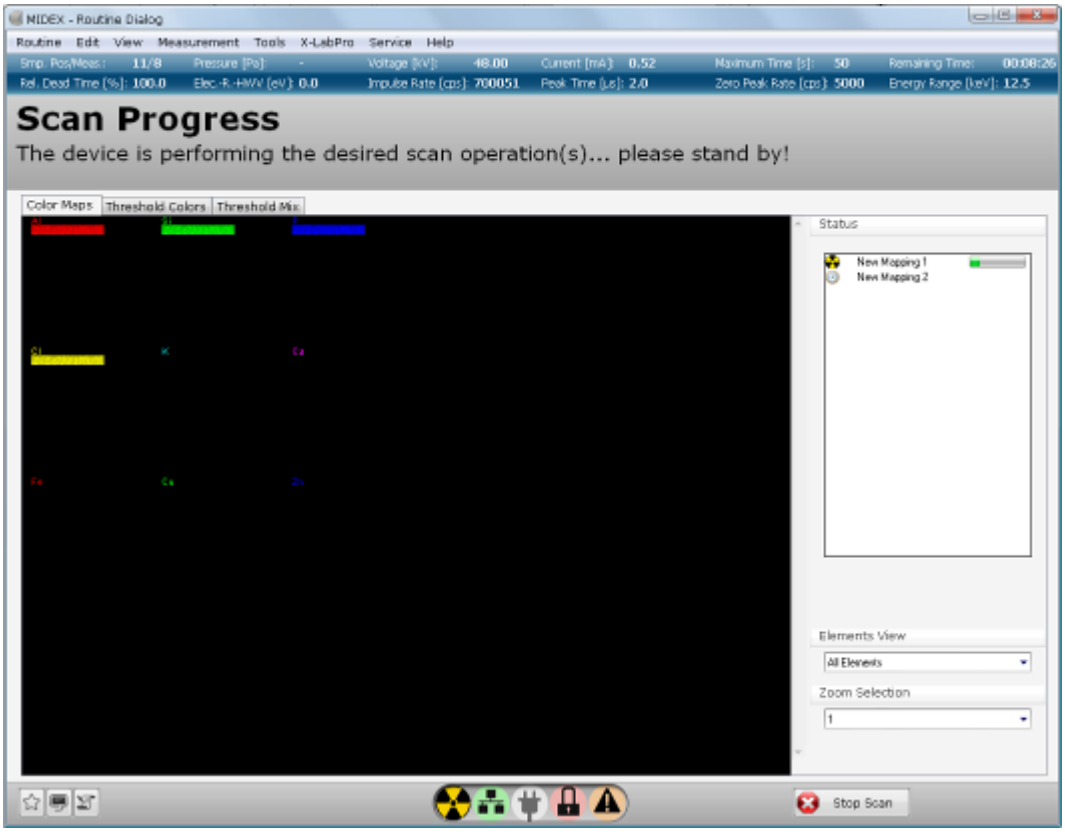
After verification of the scan setup click the **Start** button to start the scan and switch to the scan progress view.



25.6.7 Scan Progress Page

The measurement is started while switching to the scan progress dialog and will be executed automatically. No user interaction other than reviewing intermediate results is required.

During scan progress the view may switch to another result presentation as configured in your scan configuration. For more information on scan results view see chapter 4.4.7.3 Visualization of Results.



During measurement the scan progress and the remaining time is displayed in the parameters bar (see chapter 4.3.2). The X-ray generator will be active and the shutter will be opened for each scan point. The voltage of the X-ray generator will also be displayed in the parameters bar.

25.6.7.1 Display of Scan Progress

The scan progress will be displayed as remaining time of the current scan and as the amount of scans remaining to scan.

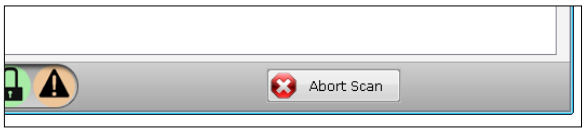
25.6.7.2 Intermediate Results View

The results displayed during measurement are not reliable. These results will be refreshed every time the detection system delivers new data. The longer the measurement process is running, the more reliable the intermediate result.

The display of intermediate results is identical to the final results view. Please see chapter 4.4.8.1 Visualization on more information.

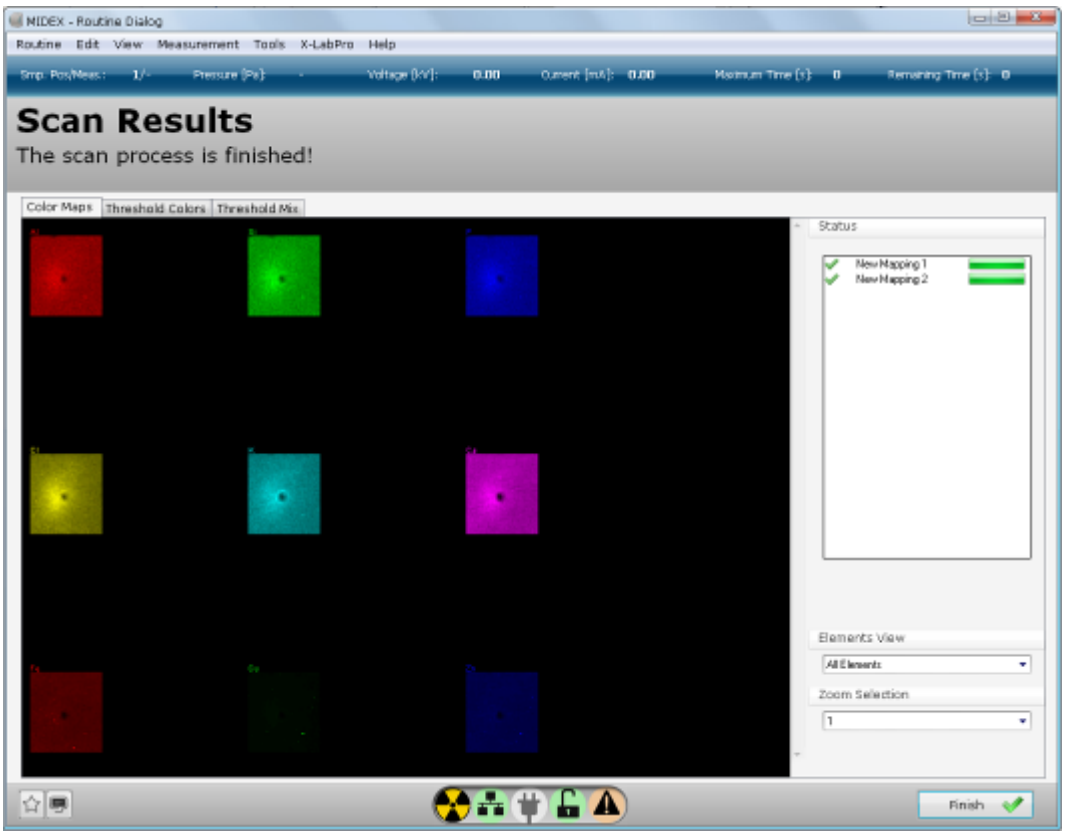
25.6.7.3 Aborting the Scan

The measurement can be aborted while it is active. To abort the measurement, click the **Abort Scan** button in the wizard navigation. All measurement data and results will be lost and the wizard will switch back to the scan setup page. Here you can correct the scan setup or go back for instance to change the sample.



25.6.8 Scan Results Page

After the automated measurement process has finished, the MIDEX Routine Dialog automatically switches to the Scan Results page. This page is identical to the scan progress page but it does not display progress information.

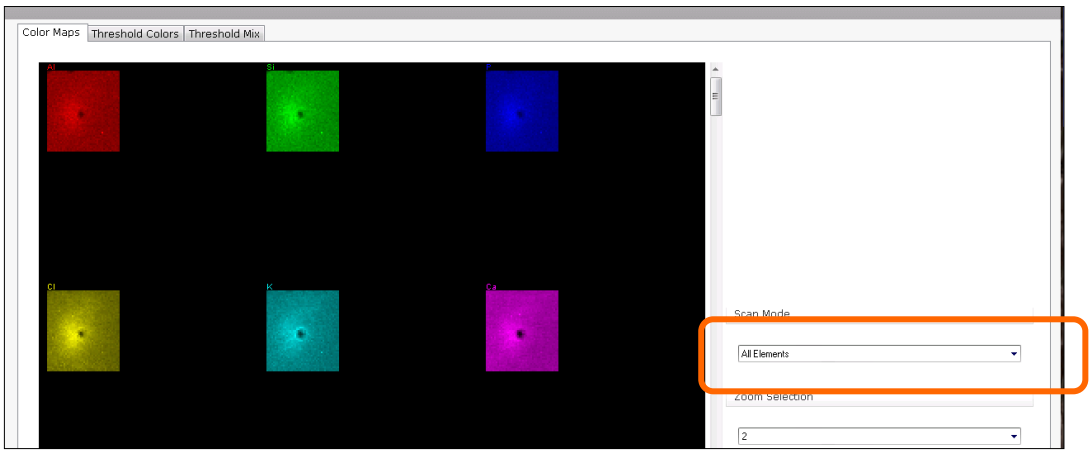


25.6.8.1 Visualization

The available visualizations depend on the scan type (Mapping, Linescan or Pointscan). Mappings can be visualized as color maps. Linescans offer Linescan view only. Pointscan results can be displayed as a list of elements or as a single spectrum. The following chapters describe these visualizations.

25.6.8.1.1 Selecting an Element

Mappings can display multiple elements in one view. These elements can be configured in the method using the X-Lab^{Pro} Method Administration.

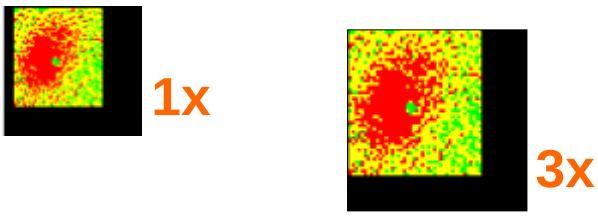


To display a single element the MIDEX Routine Dialog allows switching to a single element view. To select an element use the drop down list on the right side of the scan results page.

The **All elements** list item displays all elements configured in the method. Select an element from the drop down list and the view switches to display only the selected element.

25.6.8.1.2 Lossless Zooming of Results

A single element view can be zoomed using the **Zoom Selection** drop down list. Choose a zoom factor and the view is updated immediately. The zoom of the image is lossless, there is no interpolation. Each pixel of the Mapping will be multiplied by the zoom factor.

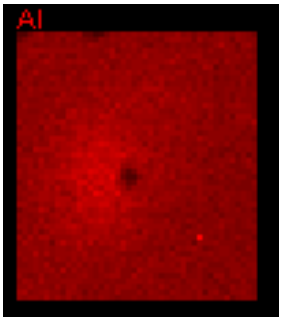


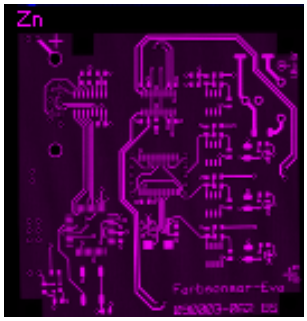
25.6.8.1.3 Color Maps

Color maps are views of the intensity of an element at a scan point (one pixel). The higher the intensity of the element, the higher gets the intensity of the color. Every element is displayed as a rectangular image with its own colors.

The base color is black, which means if the intensity gets lower, then the color of the pixel gets darker. A black pixel means the element does not exist (or the intensity is extremely low).

Here some examples from different scans:

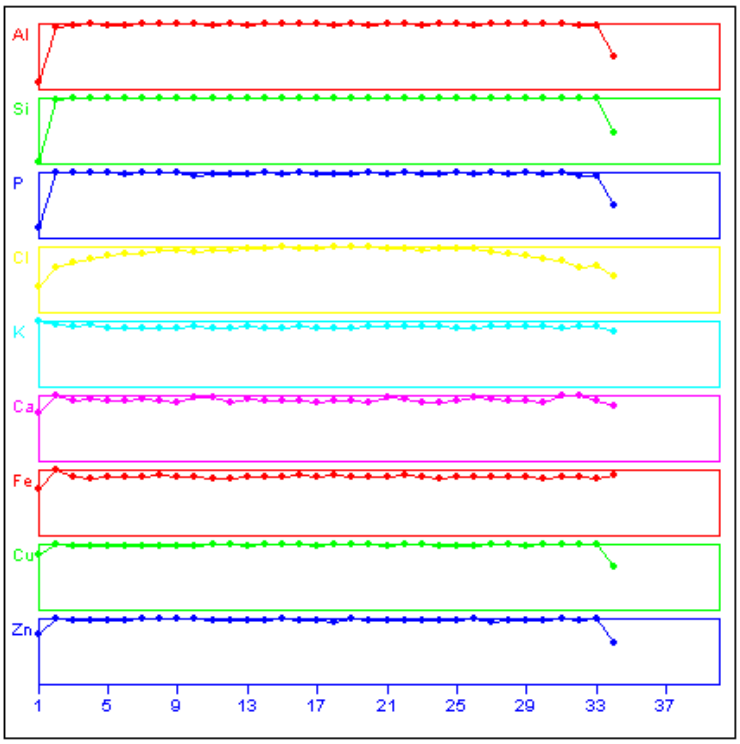




25.6.8.1.4 Linescan View

For Linescans there is only one view available. The view shows an XY graph listing the points and their relative intensity side by side. Every element is shown in a separate graph and may have a different color.

This view can be very useful to analyze the homogeneity of elements across a line on the sample. The more linear the line is displayed on the graph, the more homogeny is the element on the line.



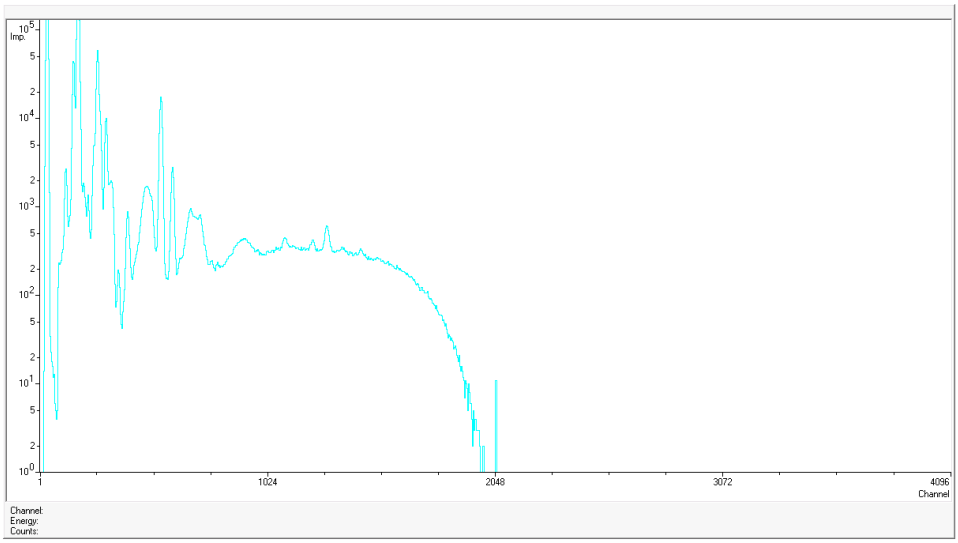
25.6.8.1.5 Result List

The result list is only available for Pointscans. It displays a list of elements and their concentrations and intensities.

Z	Sy...	Nr. of Impul...	Calc. Conc.	Unit	Abs. Error	Unit	Given Conc.	Unit	Abs. Error	Unit	L
1	H	-	0,1	µg/g	0,0	µg/g	-				
2	He	-	0,1	µg/g	0,0	µg/g	-				
3	Li	-	< 2,0	µg/g	(0,0)	µg/g	-				
4	Be	-	0,1	µg/g	0,0	µg/g	-				
5	B	-	0,1	µg/g	0,0	µg/g	-				
6	C	-	0,1	µg/g	0,0	µg/g	-				
7	N	-	0,1	µg/g	0,0	µg/g	-				
8	O	-	0,1	µg/g	0,0	µg/g	475300	µg/g	-		Cer
9	F	-	0,1	µg/g	0,0	µg/g	2100	µg/g	-		
10	Ne	-	0,1	µg/g	0,0	µg/g	-				
11	Na	17559 F	49380	µg/g	550	µg/g	48520	µg/g	-		Cer
12	Mg	2424 F	649	µg/g	33	µg/g	180,9	µg/g	-		Cer
13	Al	377531 F	78400	µg/g	150	µg/g	77800	µg/g	-		Cer
14	Si	4286154 F	329700	µg/g	200	µg/g	328800	µg/g	-		Cer
15	P	18920 F	40,0	µg/g	0,3	µg/g	61,1	µg/g	-		Cer
16	S	13344 F	214,5	µg/g	2,3	µg/g	70,1	µg/g	-		
17	Cl	-	0,1	µg/g	0,0	µg/g	180,0	µg/g	-		Cer
18	Ar	-	0,1	µg/g	0,0	µg/g	-				
19	K	115359 F	37350	µg/g	120	µg/g	37270	µg/g	-		Cer
20	Ca	12955 F	2489	µg/g	36	µg/g	2430	µg/g	-		Cer
21	Sc	-	0,1	µg/g	0,0	µg/g	0,1	µg/g	-		
22	Ti	7139 F	527	µg/g	11	µg/g	659,4	µg/g	-		Cer
23	V	0 F	< 20	µg/g	(0,0)	µg/g	3,3	µg/g	-		Cer
24	Cr	0 F	110	µg/g	110	µg/g	3,4	µg/g	-		Cer
25	Mn	6264 F	467	µg/g	14	µg/g	449,2	µg/g	-		Cer
26	Fe	220881 F	17290	µg/g	40	µg/g	17720	µg/g	-		Cer
27	Co	819 F	< 30	µg/g	(0,0)	µg/g	0,2	µg/g	-		
28	Ni	1829 F	< 20	µg/g	(0,0)	µg/g	1,5	µg/g	-		Cer
29	Cu	6494 F	< 20	µg/g	(0,0)	µg/g	4,0	µg/g	-		Cer
30	Zn	7183 F	244,5	µg/g	7,0	µg/g	224,0	µg/g	-		Cer
31	Ga	-	0,1	µg/g	0,0	µg/g	39,0	µg/g	-		Cer
32	Ge	-	0,1	µg/g	0,0	µg/g	2,3	µg/g	-		
33	As	0 F	< 15	µg/g	(0,0)	µg/g	2,3	µg/g	-		
34	Se	-	0,1	µg/g	0,0	µg/g	-				
35	Br	-	0,1	µg/g	0,0	µg/g	0,5	µg/g	-		
36	Kr	-	0,1	µg/g	0,0	µg/g	-				
37	Rb	12418 F	150,4	µg/g	2,6	µg/g	152,0	µg/g	-		Cer
38	Sr	402 F	3,4	µg/g	1,5	µg/g	3,0	µg/g	-		Cer
39	Y	17447 F	182,4	µg/g	2,5	µg/g	184,0	µg/g	-		Cer
40	Zr	79638 F	848,1	µg/g	3,8	µg/g	780,0	µg/g	-		Cer
41	Nb	-	0,1	µg/g	0,0	µg/g	110,0	µg/g	-		Cer
42	Mo	-	0,1	µg/g	0,0	µg/g	2,5	µg/g	-		
43	Tc	-	0,1	µg/g	0,0	µg/g	-				
44	Ru	-	0,1	µg/g	0,0	µg/g	-				
45	Rh	-	0,1	µg/g	0,0	µg/g	-				

25.6.8.1.6 Spectrum View

The spectrum view is only available for Pointscans. It displays the detailed spectrum received during measurement.



25.6.8.2 Result Files and Jobs

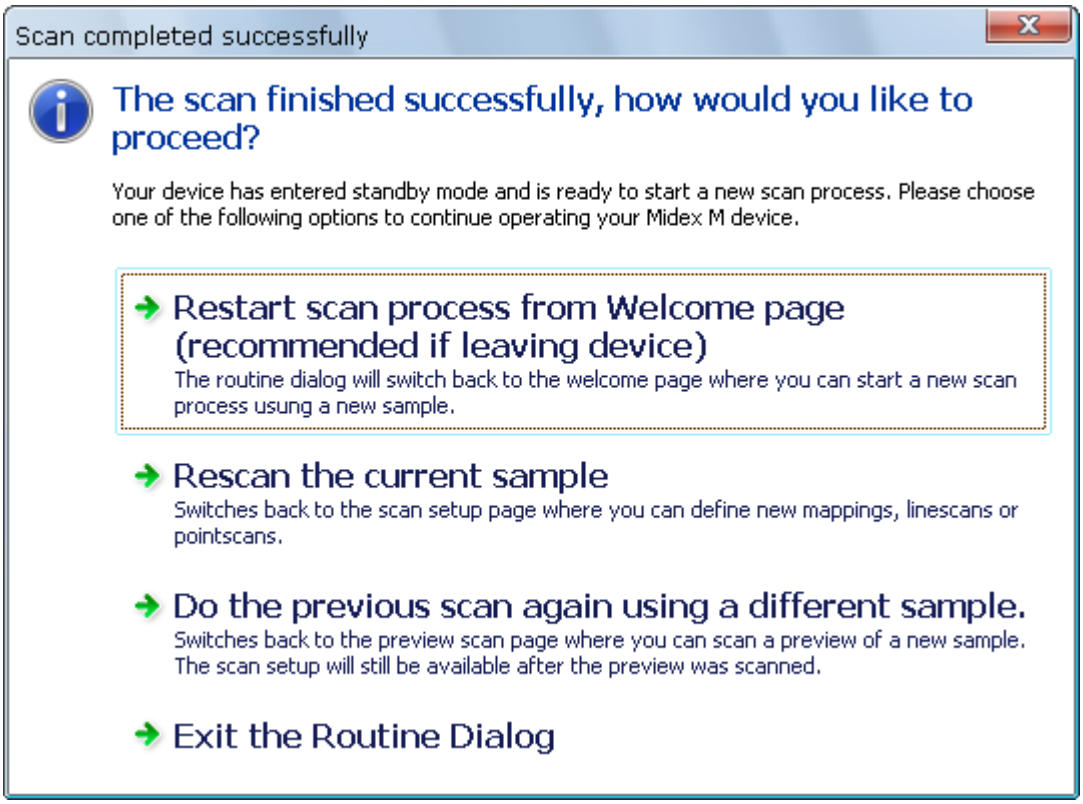
When the measurement has finished, the results are saved for later use. This is where the functionality of the MIDEX Routine Dialog ends. For further evaluation and review of results the Spectra Viewer of X-Lab^{Pro} is required.

The results of Mappings and Linescans are saved as file archives to the file system of the computer running the MIDEX Routine Dialog. Pointscans are added to Jobs and available in the X-Lab^{Pro} Job Manager.

25.7 After measurement

If the measurement was finished and the results are available, the wizard navigation displays a **Finish** button.

To finish the scan process and continue operating the MIDEX device click **Finish**. A message box will be displayed and offer different options how to continue:

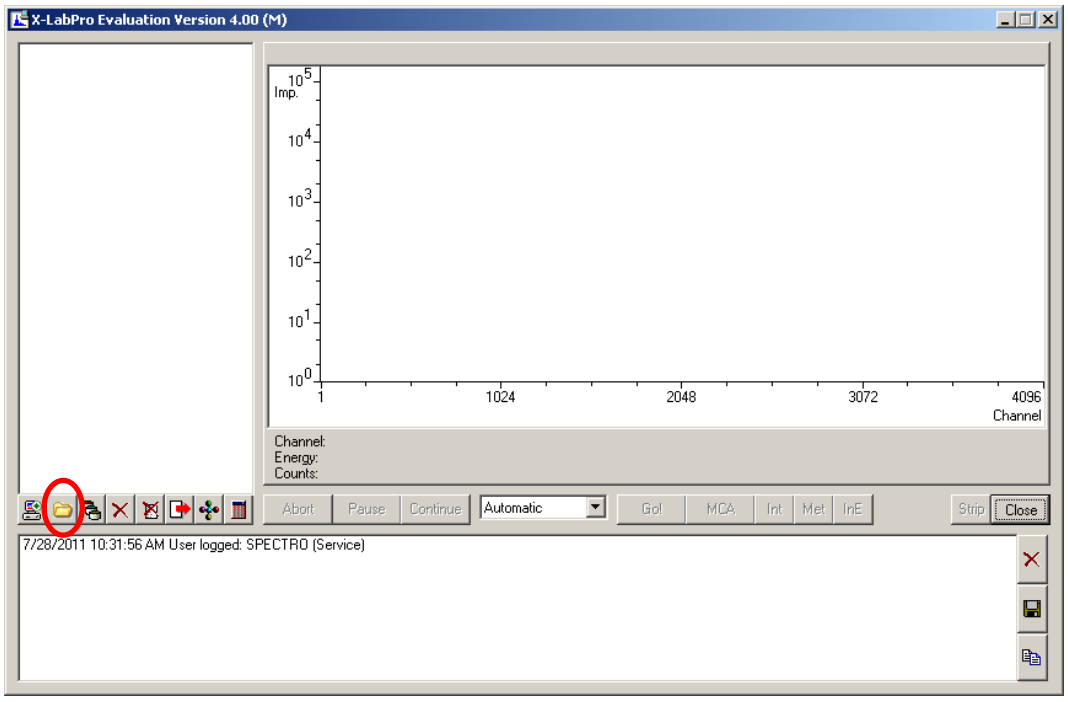

Scan completed successfully
The scan finished successfully, how would you like to proceed?
Your device has entered standby mode and is ready to start a new scan process. Please choose one of the following options to continue operating your Midex M device.
Restart scan process from Welcome page (recommended if leaving device)
The routine dialog will switch back to the welcome page where you can start a new scan process usung a new sample.
Rescan the current sample
Switches back to the scan setup page where you can define new mappings, linescans or pointscans.
Do the previous scan again using a different sample.
Switches back to the preview scan page where you can scan a preview of a new sample. The scan setup will still be available after the preview was scanned.
Exit the Routine Dialog

25.8 Evaluating of mappings measured with SPECTRO MIDEX

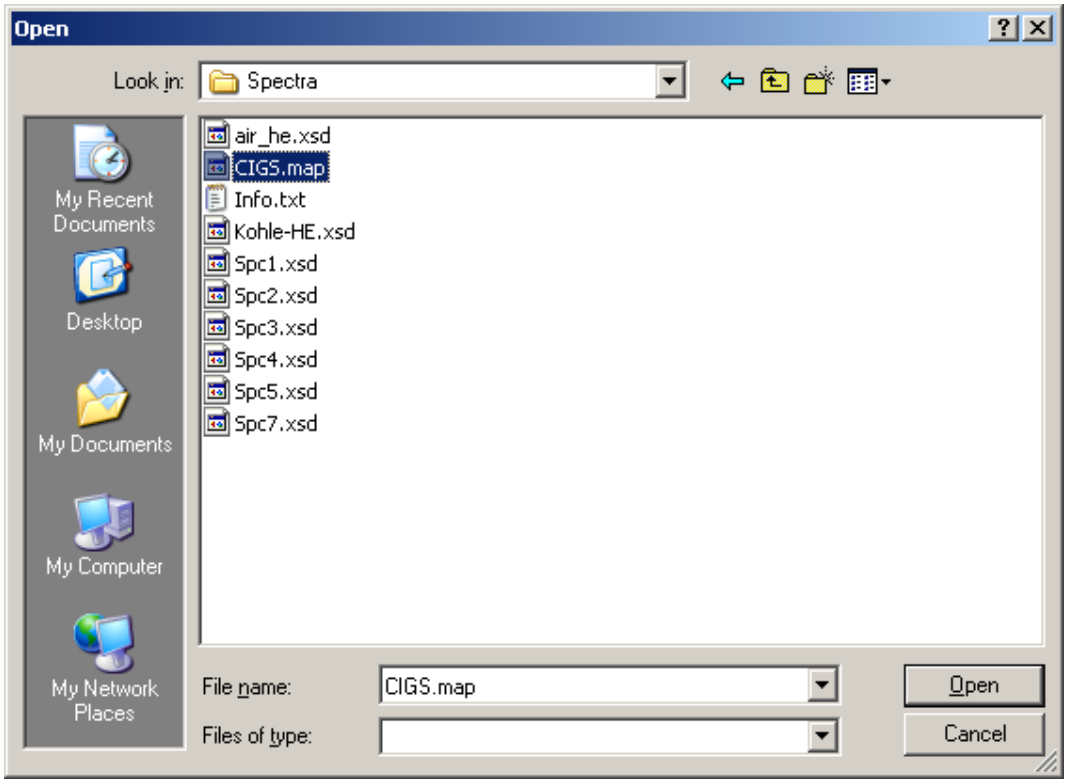
The mapping images displayed in the spectrum viewer show the intensities in regions of interest of the spectrum. In addition to this the software also allows to evaluate mapping files to get concentrations calculated and displayed in the mapping file. For this the minimum measurement time is 3 s per spectrum!

If the analytical method is already appropriate for the evaluation (for example of alloy applications) the procedure is fairly easy

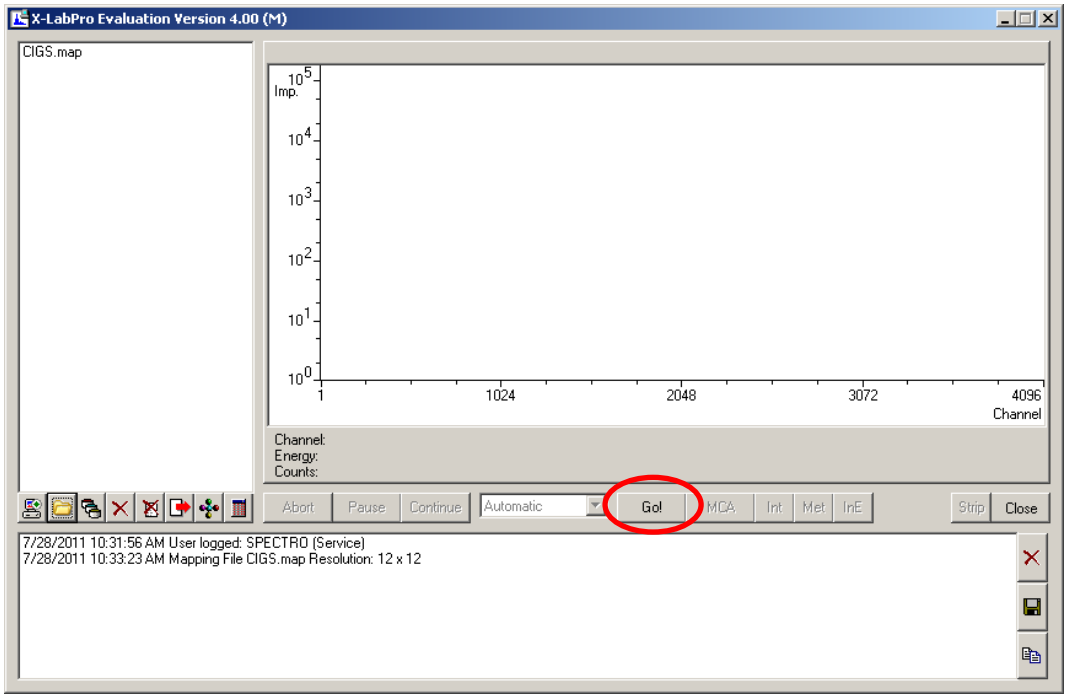
Open the evaluation tool, then click on the folder symbol to start the file open dialog.



In the following dialog select the file which shall be evaluated.



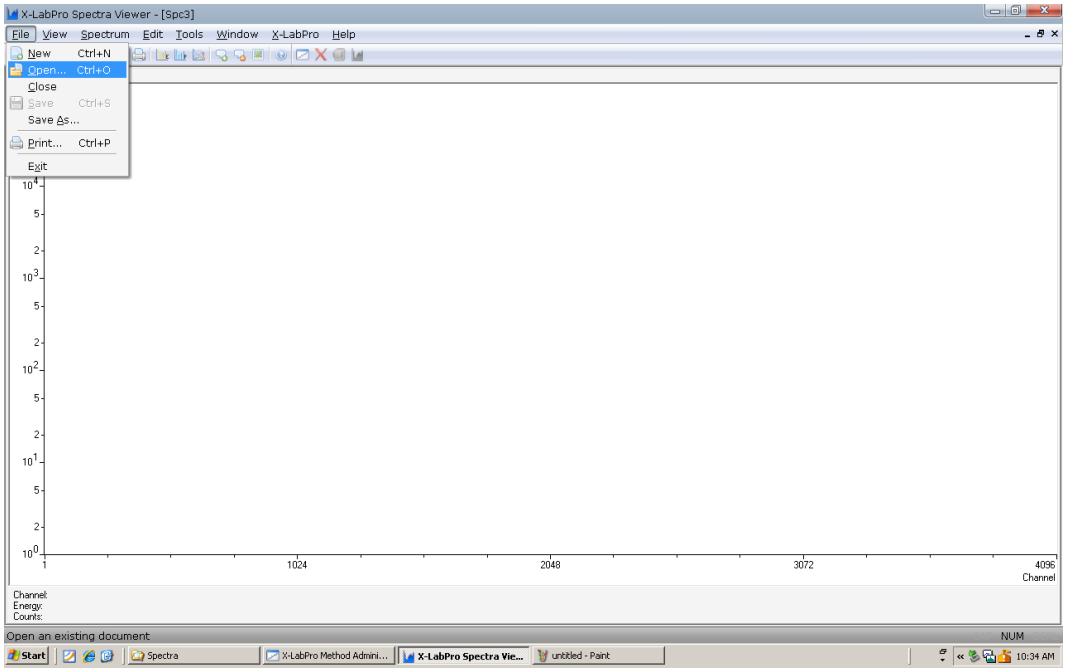
And confirm with Open. To start the evaluation click Go.

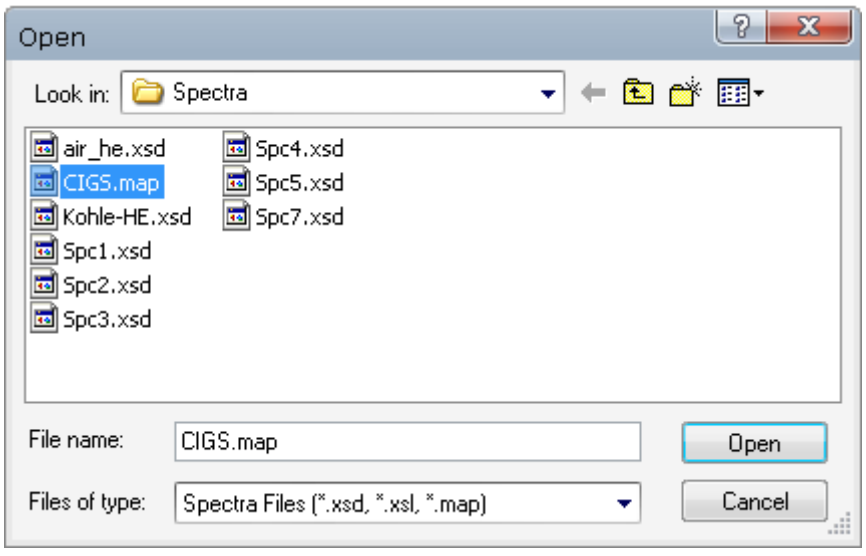


After the evaluation is finished the intensities in the mapping file will be replaced by concentration values. When opening again the mapping file in the spectrum viewer do not activate the fast evaluation when asked.

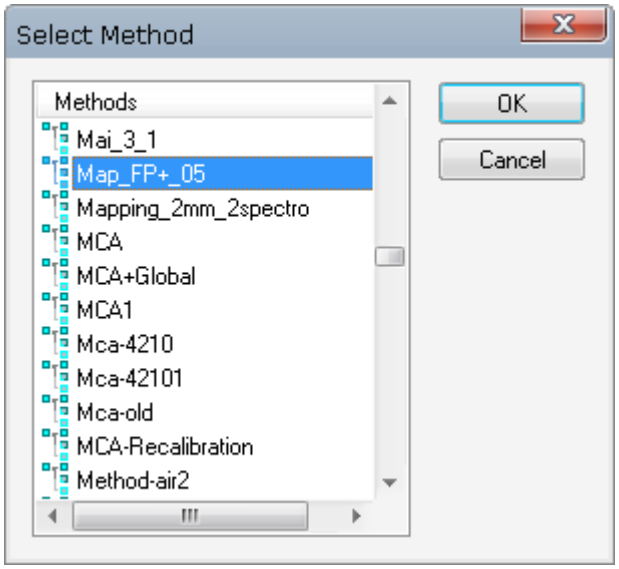
The display not contains mapping images based on concentrations. The concentrations can be exported in ASCII format with commands in the spectrum viewer window.

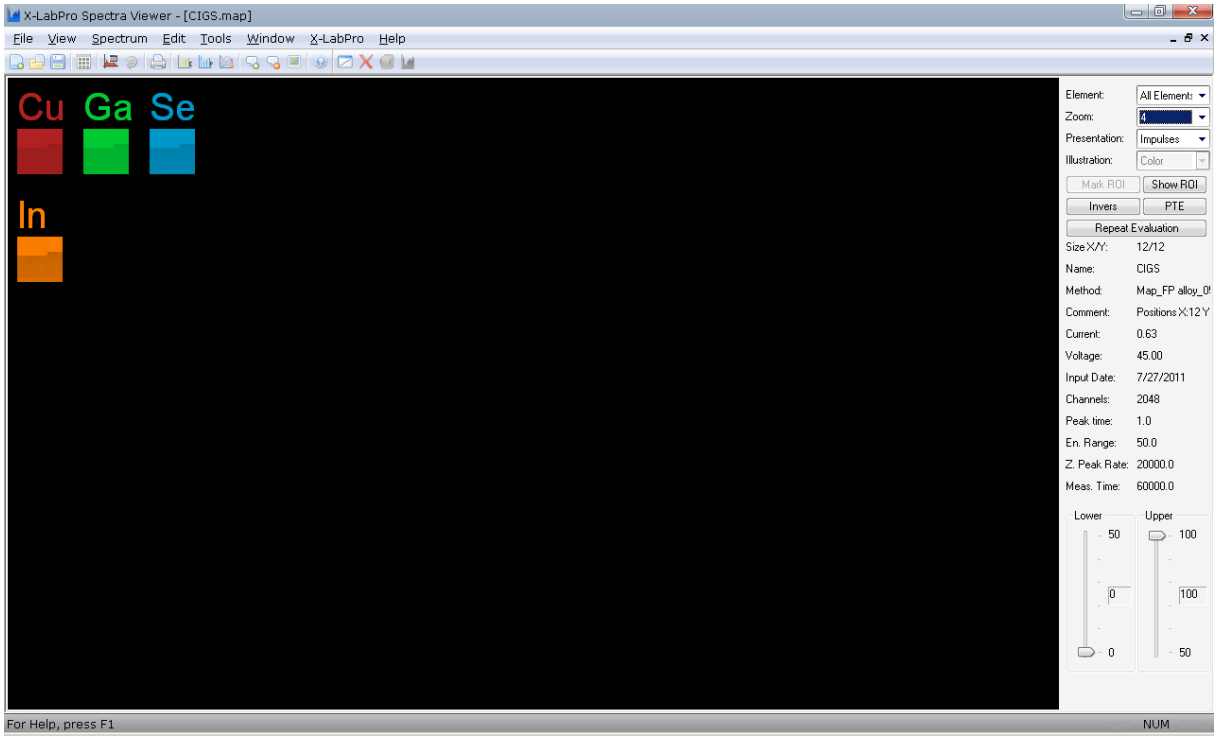
If the method is not appropriate to evaluate the mapping file or the calibration needs to be adapted the easiest way may be to create some “virtual samples” from the mapping. For this display the mapping file in the spectrum viewer.



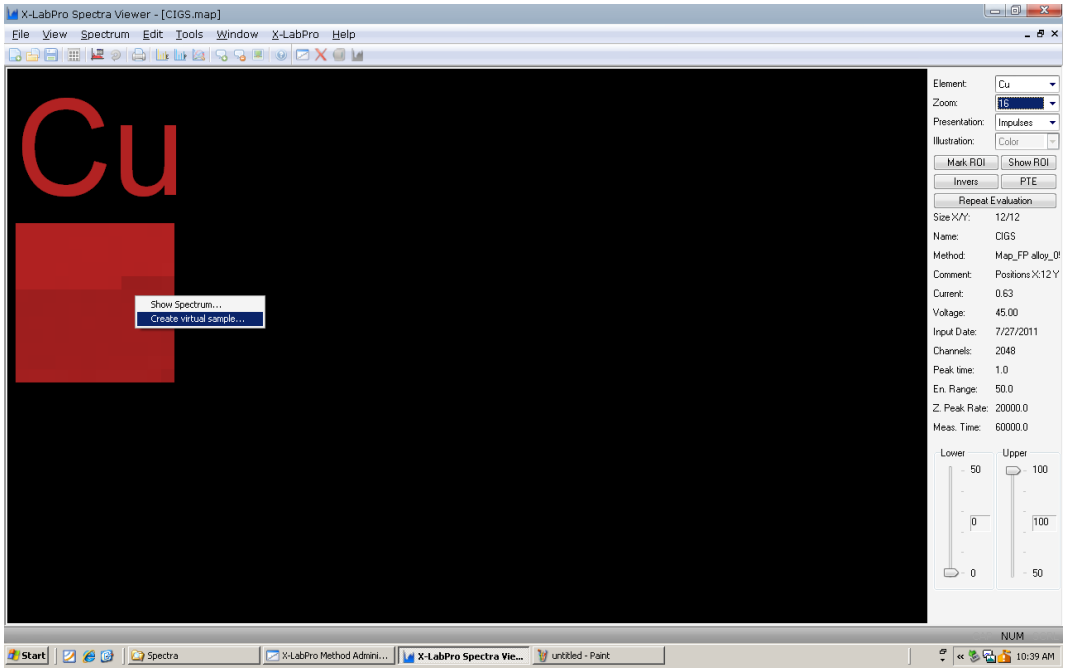


Then select the method, with which the mapping was created.

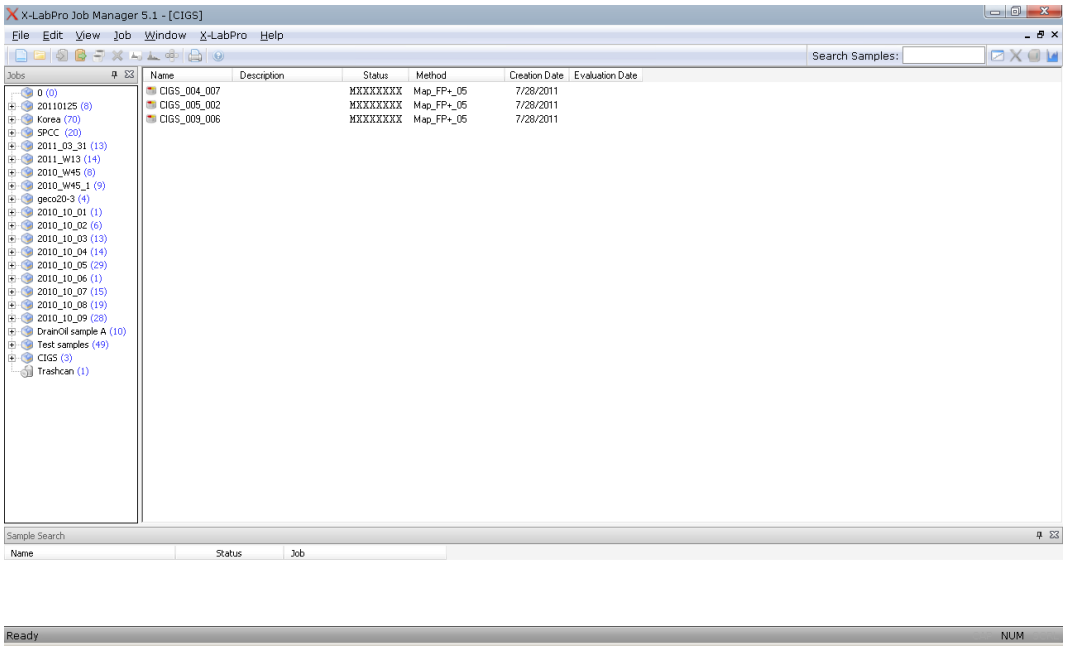




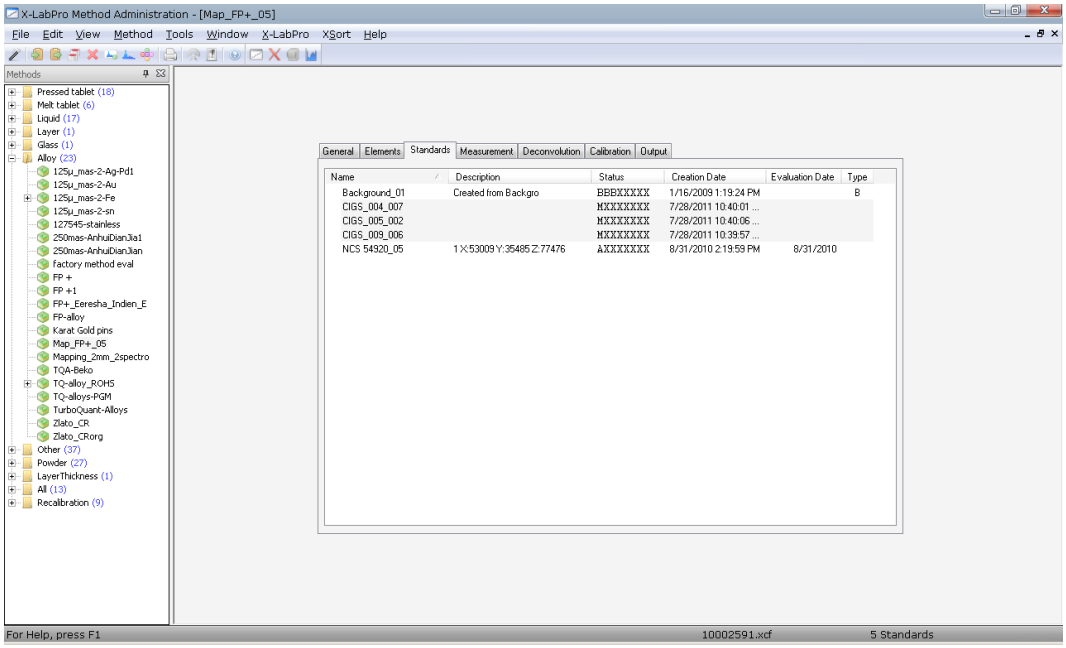
In the mapping select a single point and with a right mouse click it is possible to create a virtual sample from this single measured spectrum.



The virtual samples are stored automatically in a job with the name of the mapping file.



From here those sample files can be copied into the method.



In the method the virtual samples can be handled as “regular” samples. The calibration of the method can be changed based on the measurements of the samples.

When this procedure is finished the evaluation of the mapping file can be started as described above.

SPECTRO iQ II Easy GUI

26 How to start

To start the **X-Lab^{Pro} Easy Routine Dialog** right-click on the *Communication Server* symbol. In the upcoming menu select *Easy Routine Dialog*.

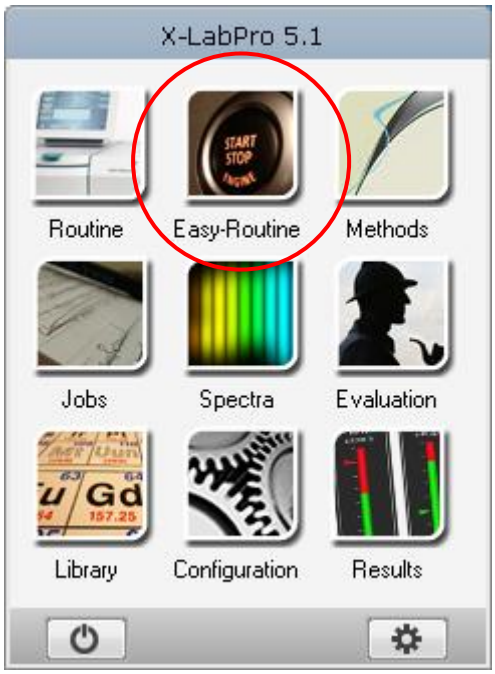


Figure 17: Using the ComServer

27 Starting up

27.1 Log in

When the **Easy Routine dialog** starts up, first you have to provide your login and password.

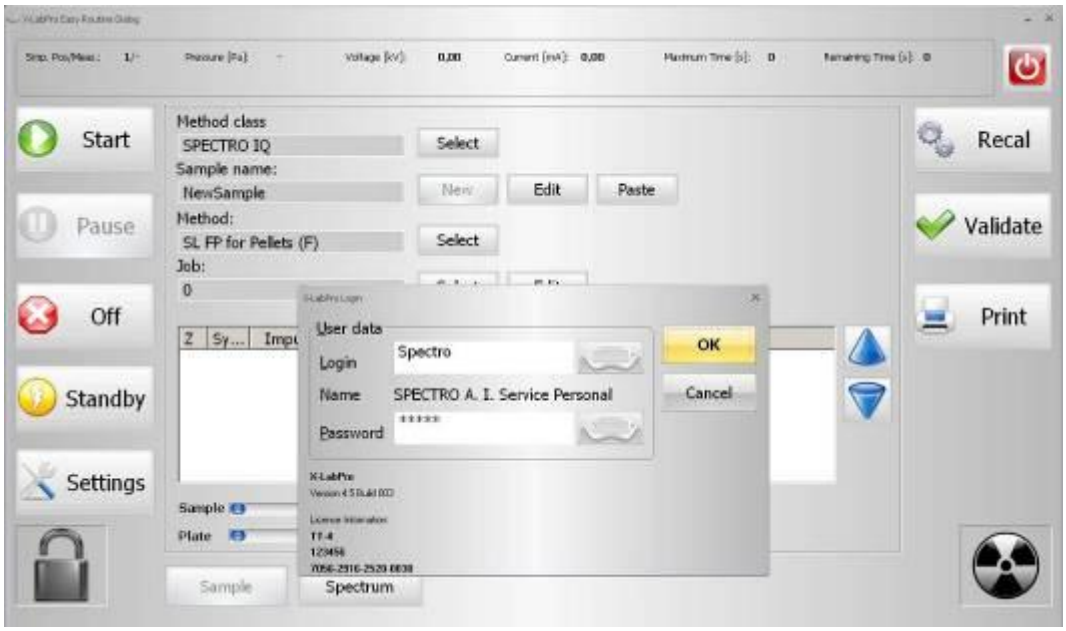


Figure 18: Log in

27.2 Interlock check

On every start up you have to perform an interlock check.

Please open the lid and close it again when you are asked for. Then press *OK*.

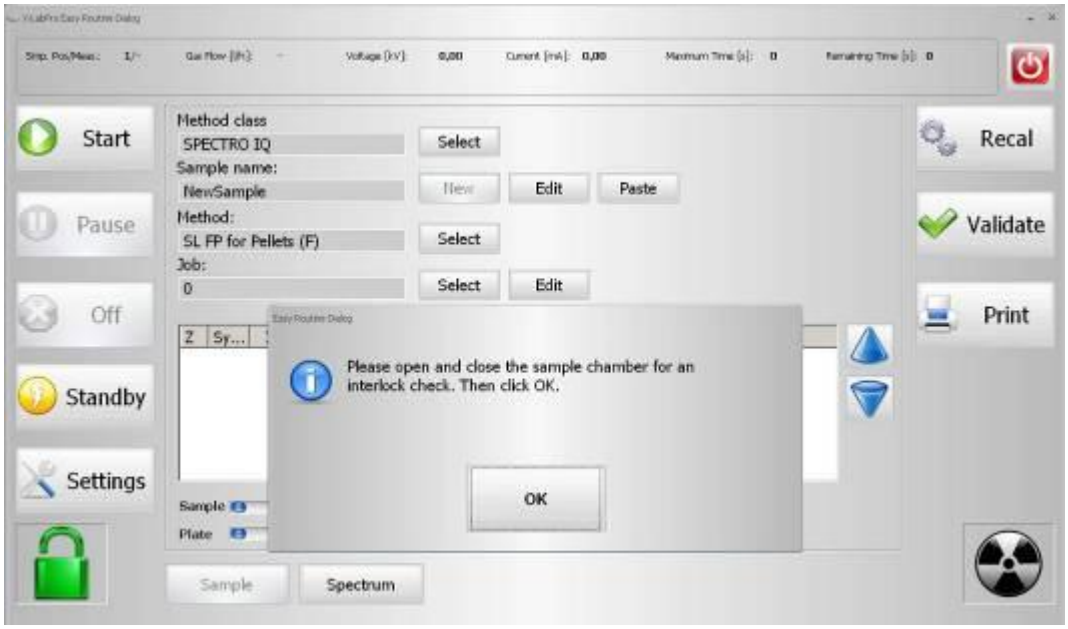


Figure 19: Interlock check

27.3 Standby mode

As next you are asked whether to go into standby mode. If you do not want to go into standby mode right now, you can switch it on later by using the *Standby button*.

28 Using Easy Routine

28.1 Introducing the dialog

When the start up procedure is finished the dialog will look like in Figure 4.

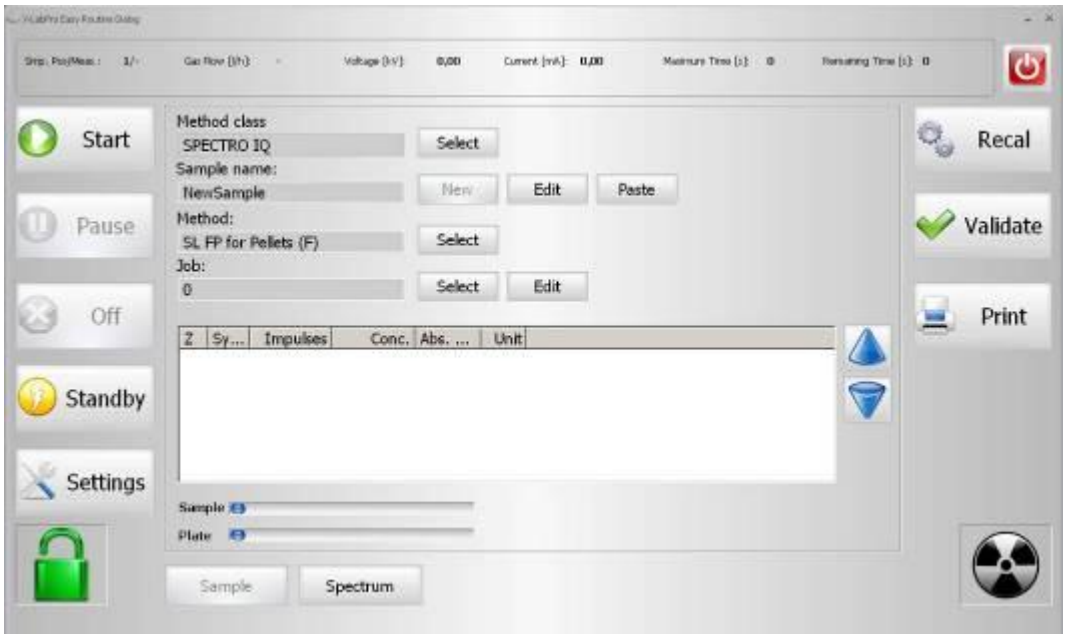


Figure 20: Easy Routine Dialog

In the upper part of the main dialog you can see the *Parameter Bar* stating the actual measurement parameters. While measuring, the bar will be updated continually.

Right next to the *Parameter Bar* is the *Close Button*.

On both sides of the dialog are several *Function Buttons*.

Below the buttons are two *State Icons*.

In the center you can see the *Sample View*. The *Sample View* is shown by default on start up. By using the buttons below the center view you can switch between *Sample View* and *Spectrum View*.

While measuring the *Spectrum View* shows the measured spectrum.

After a measurement is completed the *Sample View* shows the analysis results.

28.1.1 Sample view

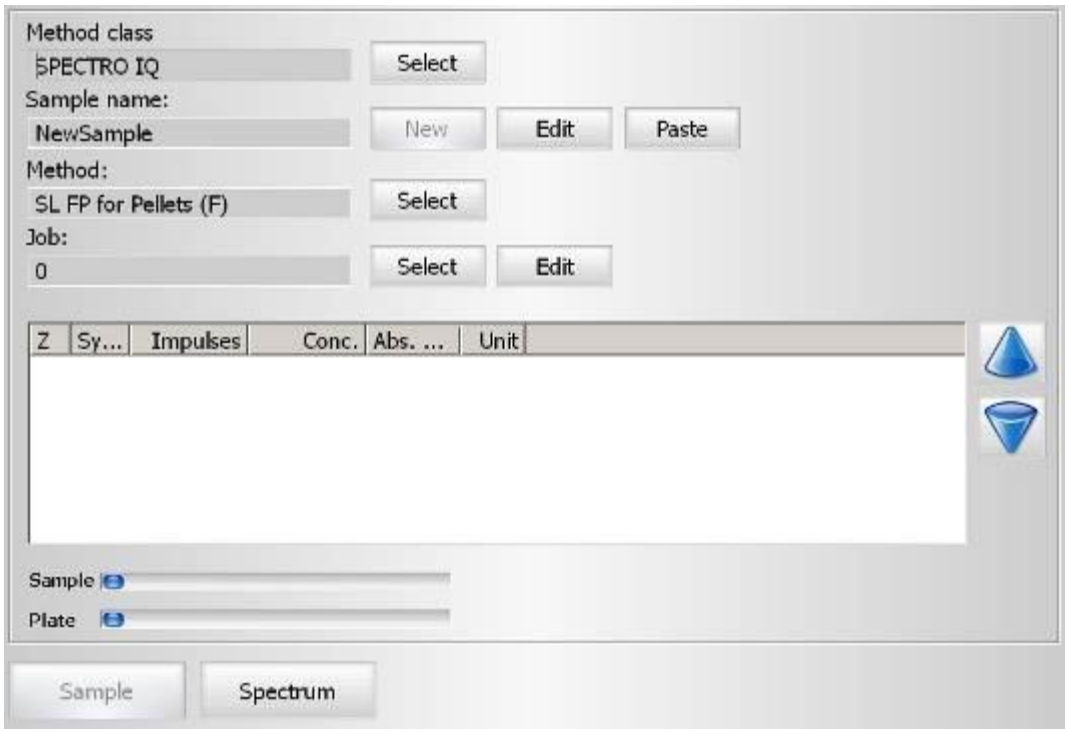


Figure 21: Sample View

The *Sample View* contains all needed controls to prepare a measurement.

In the first four rows you can edit the sample name and select the method class, method and job.

Below is the *Result List* where the measurement results are shown. After performing a *Validation* the list contains an additional row with the validation result.

The progress controls show the remaining measurement time; separated into

- Sample time: the time remaining for measuring the current sample.
- Plate time: the time remaining for the complete measuring process (incl. time for preparing a measurement with gas flush or vacuum).

The two buttons below let you switch between *Sample View* and *Spectrum View*.

28.1.2 Selecting a Method class

Press the *Select button* next to the edit field. A dialog (*Figure 6*) opens and you can select the desired method class.

28.1.3 Selecting a Method

Press the *Select button* next to the edit field. A dialog (*Figure 6*) opens and you can select the desired method.

The dialog only shows methods which are in the current method class.

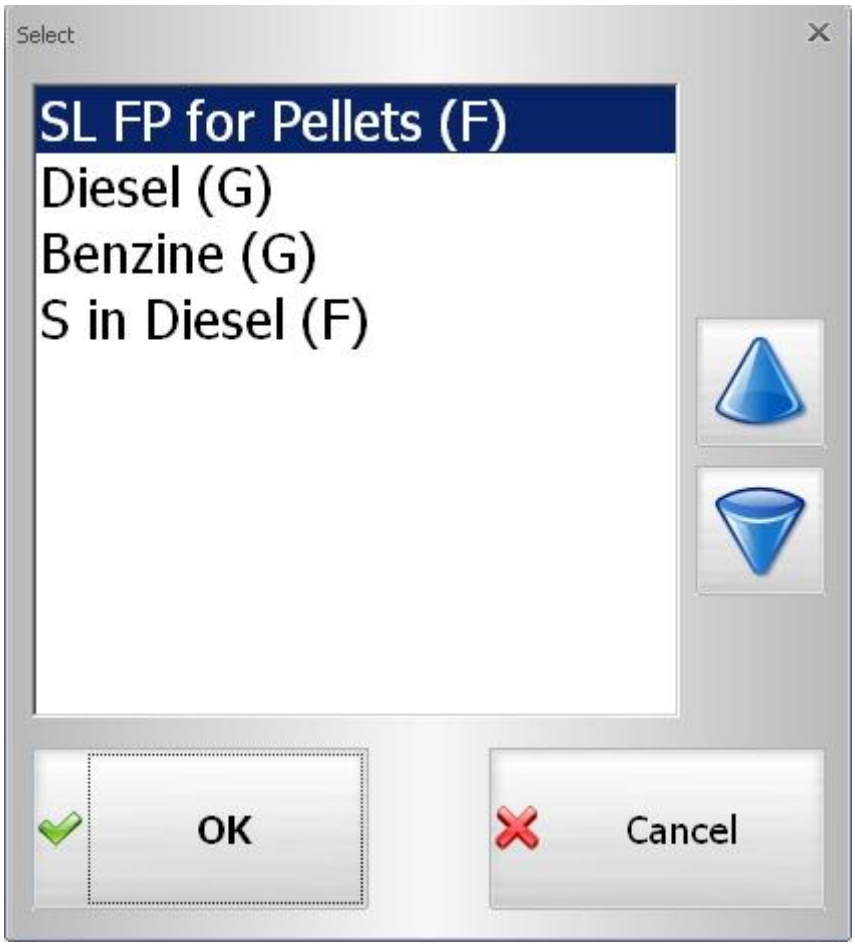


Figure 22: Select dialog

28.1.3.1 Selecting a Job

At start up the job is preset according to the setting from the Configuration Editor.

To select a different job press the *Select button* next to the edit field. A dialog (*Figure 6*) opens and you can select the desired job.

28.1.3.2 Editing a Job

To edit the job press the *Edit button* next to the edit field. A *Virtual Keyboard* (*Figure 7*) appears. Type in the new job and press OK to accept it.

28.1.3.3 Editing the sample name

At start up the sample name is preset with 'NewSample'.

To edit the sample name press the *Edit button* next to the edit field. A *Virtual Keyboard* (*Figure 7*) appears. Type in the new sample name and press OK to accept it.

28.1.3.4 Pasting a sample

Click here, to paste a sample from the *Job Manager* into **Easy Routine Dialog**.

It is not possible to paste a standard. For pasting standards, please use the **Routine Dialog**. Further on, the method to which the sample belongs must not be hidden or finalized.

It is possible to resume the measurement of a not completely measured sample. For example: if your sample contains 6 measurements and 5 of these are already measured, you can paste the sample and start measuring the last one.

It is not possible to paste a completely measured sample.

28.1.3.5 Using the virtual keyboard

Figure 23: Virtual keyboard

The *Virtual Keyboard* can be used like a normal keyboard. *Shift* and *Caps Lock* work in the expected way. Selecting characters with *Shift* is not possible.

To move the cursor in the edit field use the *Arrow buttons* left to the edit field.

To delete the character left to the cursor use the *Delete button* on the right side of the edit field.

Press *OK* to accept the name or *Cancel* to close the dialog.

28.1.4 Spectrum view

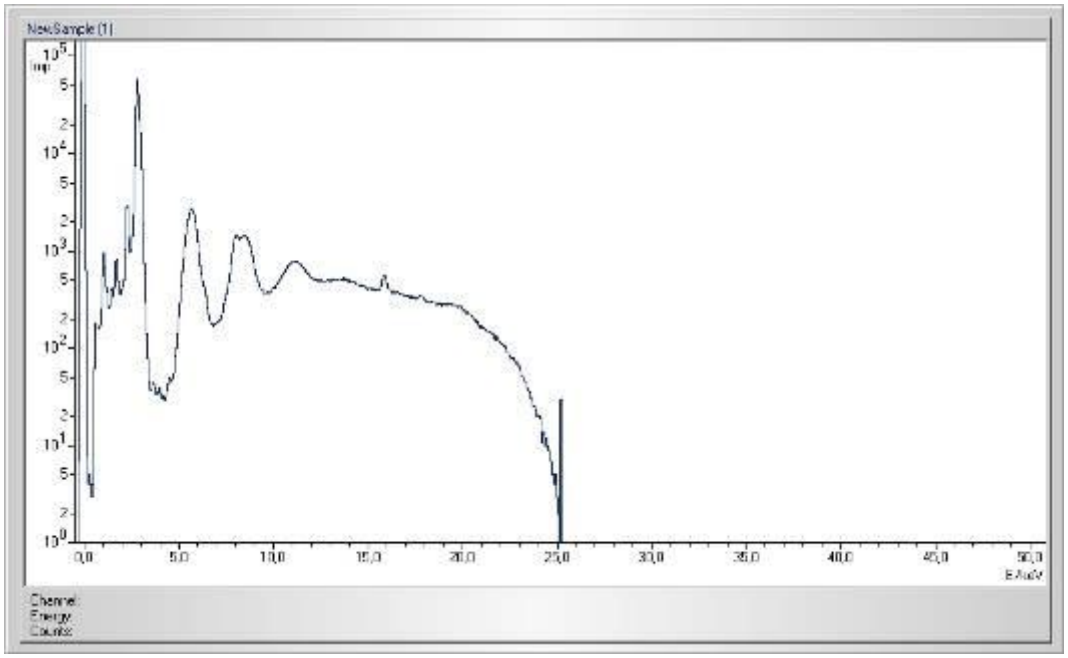


Figure 24: Spectrum View

During a measurement the *Spectrum View* displays the currently measured spectrum.

The *Spectrum View* can be enabled / disabled in the *Settings dialog*.

28.1.5 Close Button

Figure 25: Close button

Clicking the *Close button* exits the **Easy Routine Dialog**. You will have to confirm exiting. If the high voltage is switched on, it will be powered down before the dialog is closed.

28.2 Function Buttons

28.2.1.1 Start

Figure 26: Start button

The *Start button* is active only when no measurement is performed.

Clicking the *Start button* starts a new measurement.

It will change into the *Stop button* while measuring.

28.2.1.2 Stop

Figure 27: Stop button

The *Stop button* appears only during measurements.

Clicking the *Stop button* stops the actual measurement. The high voltage will stay switched on. When the measurement is stopped, the *Start button* is shown again.

28.2.1.3 Pause

Figure 28: Pause button

The *Pause button* is active only during a measurement.

Clicking the *Pause button* will pause the measurement.

It will then change into the *Continue button*.

28.2.1.4 Continue

Figure 29: Continue button

The *Continue button* appears only during paused measurements.

Clicking the *Continue button* will continue a paused measurement. When the measurement is continued the *Pause button* is shown again.

28.2.1.5 Off

Figure 30: Off button

The *Off button* is active only when the x-ray tube is on.

Clicking the *Off button* ends the **Standby mode**.

28.2.1.6 Standby

Figure 31: Standby button

The *Standby button* is active only when the x-ray tube is off.

Clicking the *Standby button* switches the instrument into **Standby mode**.

28.2.1.7 Settings

Figure 32: Settings button

The *Settings button* is active only when no measurement is performed.

Clicking the *Settings button* opens the *Settings dialog* (see chapter **Settings dialog** for more details).

28.2.1.8 Recalibration

Figure 33: Recalibration button

The *Recalibration button* is active only when no measurement is performed.

Clicking the *Recalibration button* opens the *Recalibration dialog* (see chapter **Recalibration dialog** for more details).

28.2.1.9 Validate

Figure 34: Validate button

The *Validate button* is active only when no measurement is performed.

Clicking the *Validate button* to prepare a validation. In the upcoming dialog you have to select which method contains the needed *Validation Sample*. After successfully selecting the method, click *Start* to perform the validation.

28.2.1.10 Print

Figure 35: Print button

The *Print button* is active only when no measurement is performed.

Clicking the *Print button* will print the actual measurement results directly to the default printer. When no results are present nothing is printed.

28.2.2 Parameter Bar

Figure 36: Parameter Bar

The *Parameter bar* states the actual measurement parameters:

- the part measurement of the actual sample.
- the gas flow in liters per hour.
- the voltage in kilovolts.
- the current in milliampere.
- the maximum measurement time for the part measurement of the sample in seconds.
- the measurement time for the part measurement of the sample in seconds.

28.2.3 State Icons

The *State icons* reflect the actual instrument state. Therefore each icon has two different states.

28.2.3.1 Lock/Unlock

Figure 37: Sample chamber locked

The sample chamber is locked.

Figure 38: Sample chamber accessible

The sample chamber is accessible.

28.2.3.2 X-Ray on/off

Figure 39: X-Ray on

The x-ray tube is switched on.

Figure 40: X-Ray off

The x-ray tube is switched off.

28.2.4 Settings dialog

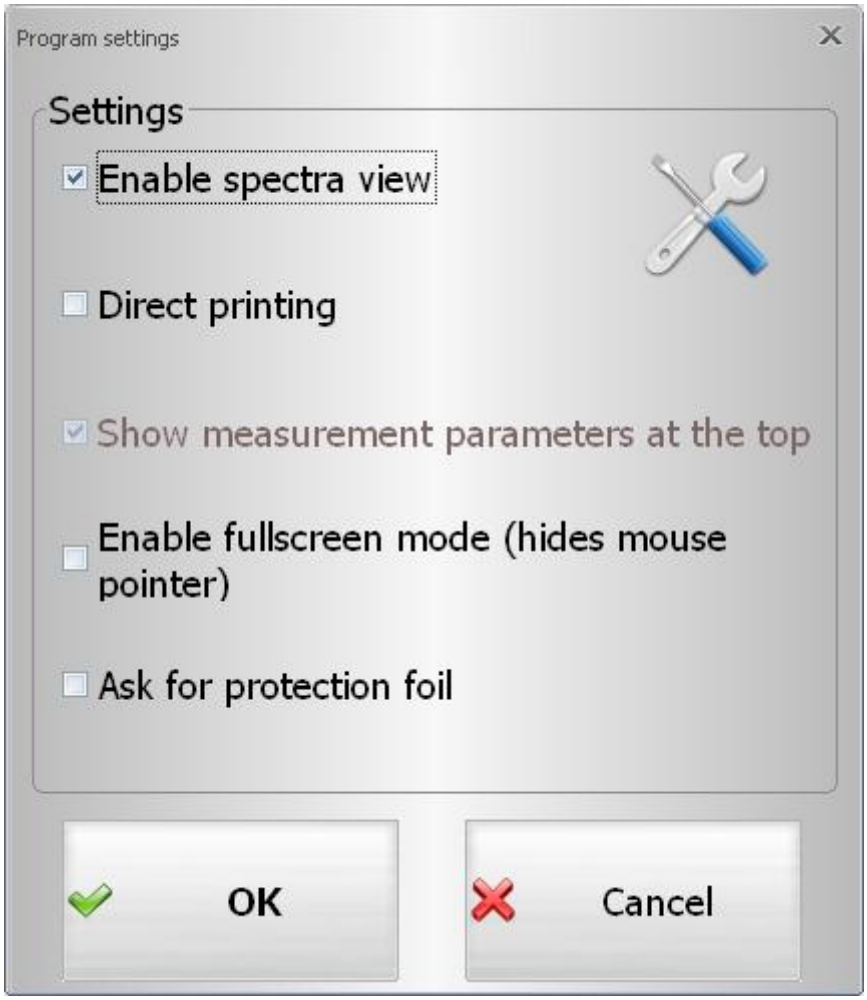


Figure 41: Settings dialog

The *Settings dialog* lets you configure some parts of the **Easy Routine dialog**.

- enable / disable the Spectrum view.
- enable / disable printing directly after evaluation of the measurement.
- enable / disable *Full screen mode*. The *Full screen mode* is suitable only when a touch screen monitor is used because in *Full screen mode* the mouse pointer is hidden.
- enable / disable the question for an inserted protection foil.

28.2.5 Recalibration dialog

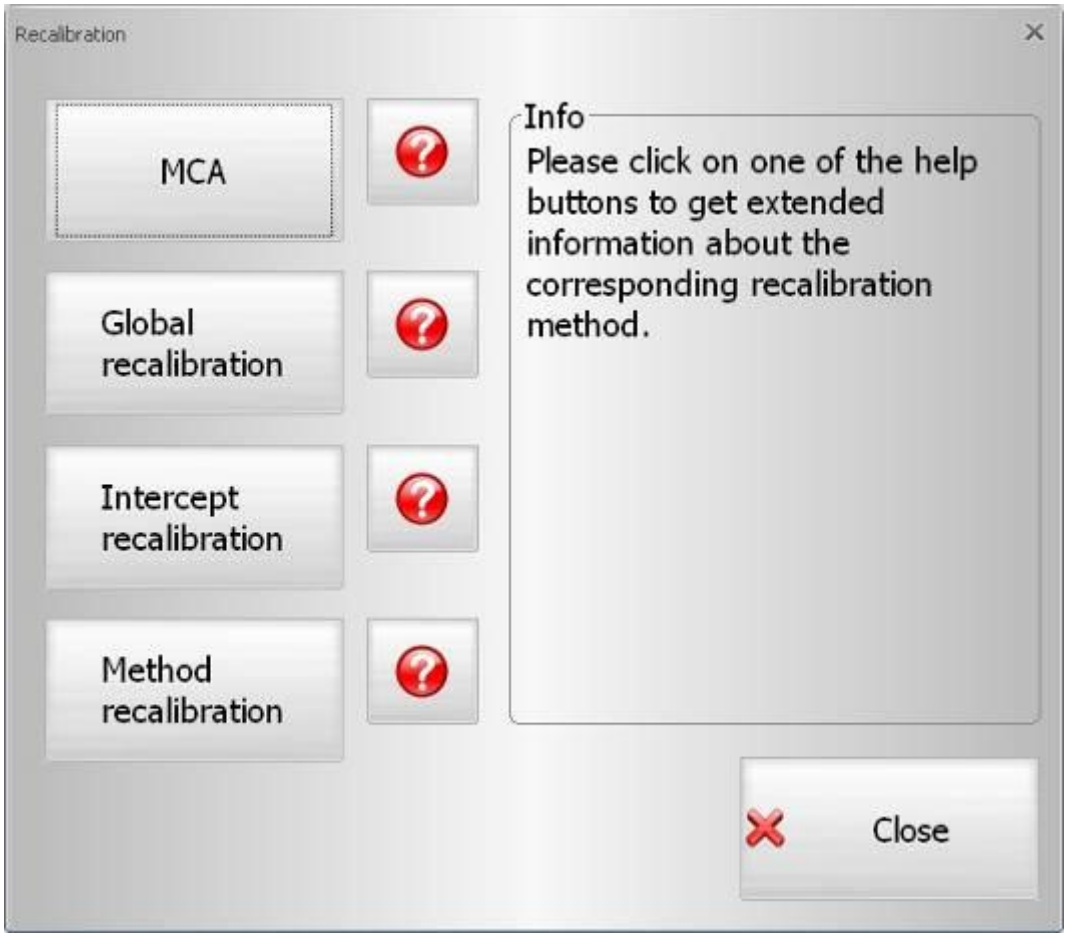


Figure 42: Recalibration dialog

With the *Recalibration dialog* you can prepare the instrument calibration.

Click one of the *Recalibration method buttons* to prepare the recalibration.

For information about the different calibration methods click the *Help button* next to the *Recalibration method button*.

28.3 Recalibration

In this chapter the application flow of the different recalibration methods is explained.

For information about the different calibration methods open *Recalibration dialog* and click the *Help button* next to the *Recalibration method* you are interested in.

28.3.1 MCA

To perform a **MCA Recalibration**, open the *Recalibration dialog* and click the *MCA button*. The recalibration is then prepared. If the actual method does not contain any *MCA sample* you will be noticed.

If a *MCA sample* was found, the **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

When the recalibration is complete the results are shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

28.3.2 Global

To perform a **Global Recalibration**, open the *Recalibration dialog* and click the *Global Recalibration button*. The recalibration is then prepared. If the actual method does not contain any *Global sample* you will be noticed.

If a *Global sample* was found, the **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

Depending on the settings in the **Configuration Editor** the **Global Recalibration** is performed with one or more samples.

If more than one sample is calibrated, a message box advises you when to insert the next sample into the **Sample Chamber**.

When the recalibration is complete the results are shown in the *Result List*. If more than one sample was measured, the results are only written to file and nothing will be shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

28.3.3 Intercept

To perform a **Intercept Recalibration**, open the *Recalibration dialog* and click the *Intercept Recalibration button*. A *Select Dialog* opens and you can choose a method for calibration. The method must contain an *Intercept Sample*. After successfully selecting a method, the recalibration is then prepared.

The **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

Depending on the settings in the **Method Configuration** the **Intercept Recalibration** is performed with one or more samples.

If more than one sample is calibrated, a message box advises you when to insert the next sample into the **Sample Chamber**.

When the recalibration is complete the results are shown in the *Result List*. If more than one sample was measured, the results are only written to file and nothing will be shown in the *Result List*. The **Easy Routine Dialog** switches back to *Normal Mode*.

28.3.4 Method

To perform a **Method Recalibration**, open the *Recalibration dialog* and click the *Method Recalibration button*. A *Select Dialog* opens and you can choose a method for calibration. The method must contain a *Method Sample*. After successfully selecting a method, the recalibration is then prepared.

The **Easy Routine Dialog** then switches into *Recalibration Mode*: only the *Start button* and the *New Sample button* are active. To perform the recalibration click *Start*. To cancel the recalibration click *New Sample*.

When the recalibration is complete the results are shown in the *Result List*. In an additional column in the *Result List* the recalibration factors are shown.

The **Easy Routine Dialog** switches back to *Normal Mode*.

28.4 Validation

In this chapter the application flow of the validation is explained.

To perform a **Validation**, click the *Validation button*. A *Select Dialog* opens and you can choose a method for validation. The method must contain a *Validation Sample* against which the new sample is validated. After successfully selecting a method, the **Validation** is then started.

When the **Validation** is complete the results are shown in the *Result List*. In an additional column in the *Result List* the validation result is shown:

- a marks a valid result, the measured concentration was within limits.
- a marks an invalid result, the measured concentration was out of range.

The **Easy Routine Dialog** switches back to *Normal Mode*.

SPECTRO iQ II XRF Tutorial

29 Method Administration

The term *method* is used in a very specific way in the X-LabPro Software. A *method* is far more than only a calibration.
It is a complex structure built up from sub-methods:

The Method Administration is divided into different parts:

- General
- Elements
- Standards
- Measurement
- Deconvolution
- Calibration
- Output

In *General* all general parameters can be found.

In *Elements* the elements for the calibration (and additional elements, which can be in the samples) are selected. In addition the concentration range is defined here.

The card *Standards* contains a list of all standard samples in this method. This list is used to create standards, to define the given concentrations...

Measurement defines all parameters of the *measurement*: the x-ray tube conditions (voltage and current), type of sample, evacuation of the sample chamber, measuring time, target, and so on.

The *deconvolution* section defines the elements of interest for each target / measurement.
During the *deconvolution* the net count rates for the selected elements are determined.

The *calibration* contains the functions typically described by the term calibration. The selection of a specific calibration model and the correlation between net count rates and concentrations are part of this sub-method.

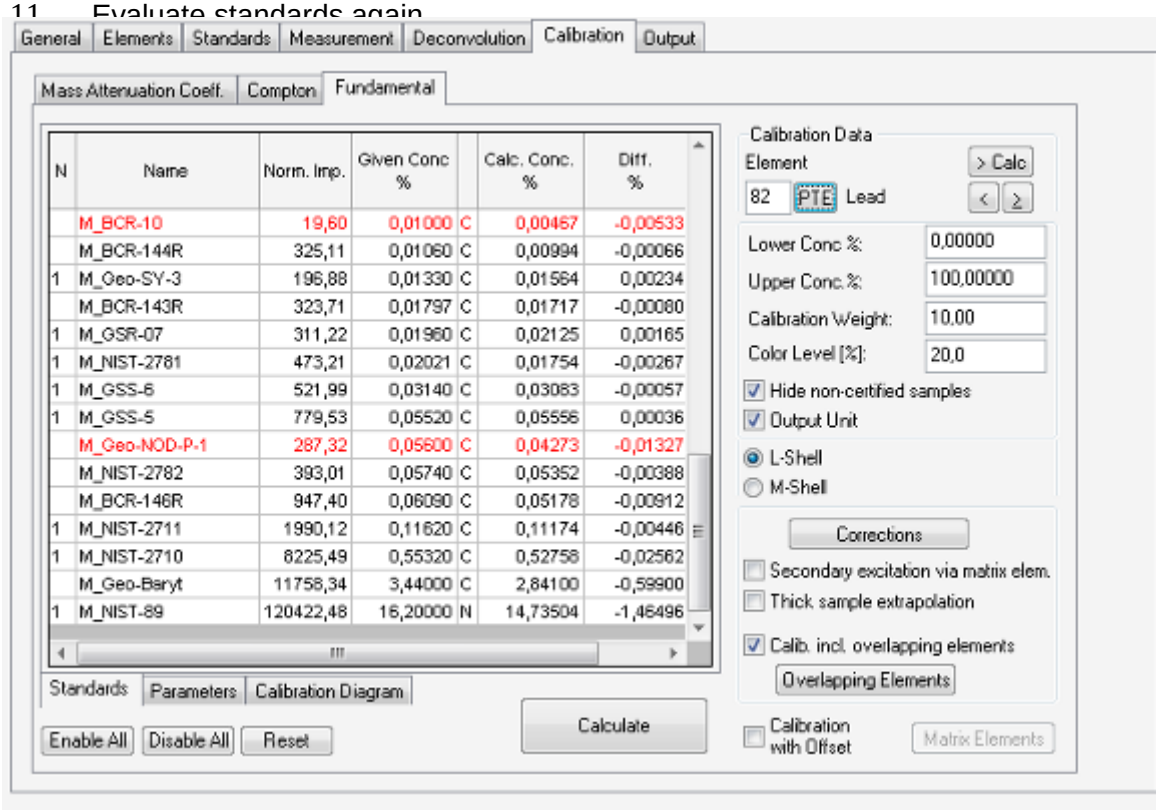
This options and cards can be used to modify or check an existing method.

To *create a new method*, a comparable method should be selected in the tree part of the screen. This source is copied using *New* in the menu Method. The visible method is copied (with or without samples can be chosen in the following window). That is the best way to start, because a method contains a lot of parameters and details and all these will be copied from a working method. That's much easier then start to start all over.

"How to create a new Method?" descibes the sequence of the most important steps. In addition to this way, the Method Wizard can be a help to accelerate this.

The a.m. parts are influenced by each other, and the best way to design a new method is to start with *elements*, followed by the *measurement*, the *deconvolution*, the *calibration* and finished with the *output*.
But even the first steps, the selection of elements and the measurement conditions, are already influenced by the aims of the calibration. A brief outline of the steps for an idealized method development is listed below:

1. Select the Elements, which can be in the samples
2. Select the Elements, for which a concentration should be calculated (they have to be a part of the elements selected one step above)
3. Depending on 1. and 2. the Measurement Conditions have to be selected
4. Measure one or several standards without evaluation and use the Spectra Viewer to check 1. - 3.
5. Optimise the measurement conditions depending on the results of 4.: This can be: Vacuum?, gas-flush?, measurement time? or excitation conditions?
6. Define or optimise the deconvolutrion parameters based on 1. and 2.
7. Measure the calibration standards
8. Optimise background spectra for the method
9. Evaluate the samples to get the net count rates
10. Calibrate the method. The procedure, which should be used, depends on the number of elements and the concentration range
11. Evaluate standards again



This figure above shows the calibration screen, when the SPECTRO procedure is selected. This is the most comprehensive calibration and contains three different sub-procedures:

- Mass Attenuation Coefficient This procedure is used to calculate the "concentration"
  of the non-visible part of the sample. This calculation - based on the Compton-peak - is used to normalize the results (of an unknown sample). Whether this feature can be used, depends on the selected procedure. Whether it should be used, can be defined in General.
- Compton Calibration This calibration is an empirical calibration. As part of the SPECTRO procedure, it is used to calculate start values for the following and final calibration based on Fundamental Parameters.
  The Compton model is using the intensity of the scattered Compton peak to correct matrix influences.
- Fundamental Parameter Calibration. The Fundamental Parameter Model (FP) is a calibration model, which tries to explain the spectra of the sample by physical equations. At the end of this procedure, a theoretical sample is calculated, which shows the same spectra as the measured one.
- On top of this selection list an important and well-known calibration can be chosen:
  Lucas-Tooth, Price. This calibration is the easiest correlation between intensity and concentration, because it's a line, described by *concentration = calib-factor * intensity*.

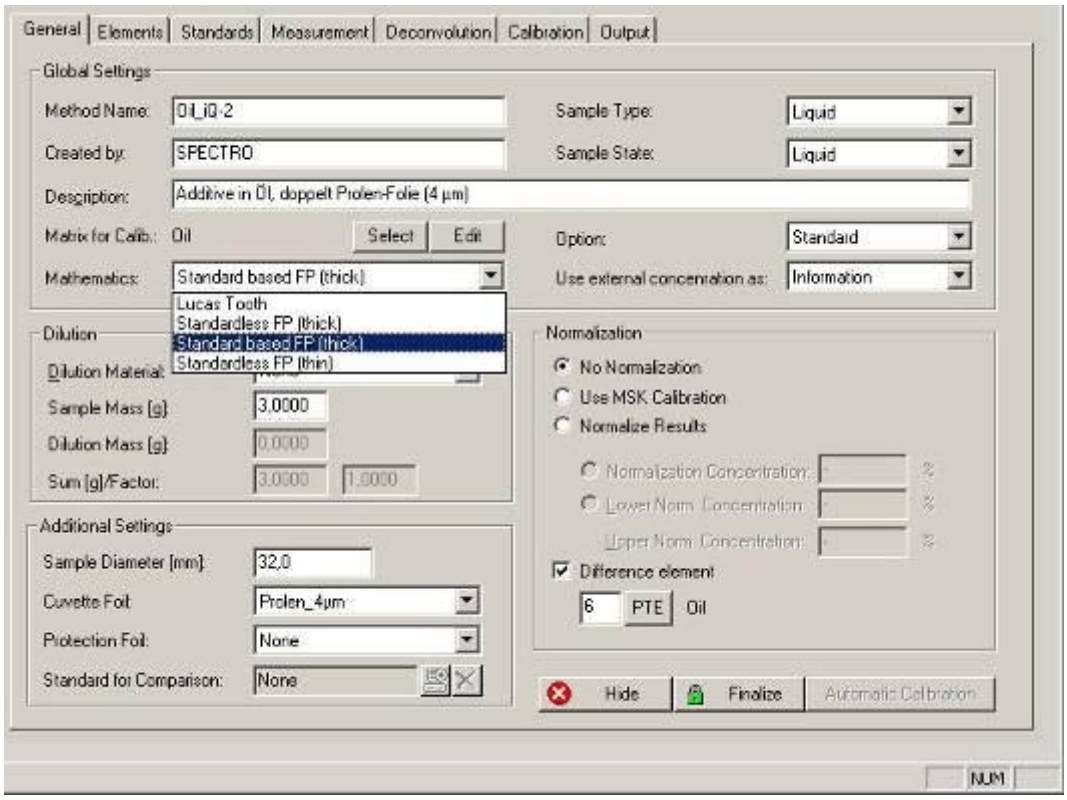
As **summary**, three analytical procedures (plus combinations for hybrid procedures) can be used in X-Lab^{Pro}:

- Lucas-Tooth, Price as easiest calibration model
- Extended Compton model using the Compton peak for matrix correction, if the concentration range is too wide for Lucas-Tooth/Price
- Fundamental Parameter Model, if the concentration range (and the matrix range) is wide

30.1 Calibration Procedure

The sub-method *Calibration* is used to get the correlation between the measured net count rates and the given concentrations of the standards. The simplest case is a linear relation between these two values, but in most cases it will be more complex. In X-ray fluorescence, the net count rate is influenced drastically by the matrix and therefore needs an evaluation model to correct for this.

The software X-LabPro contains a wide selection of calibration models. They can be selected using the function *Mathematics* in the tab *General*.



The Calibration models can be divided into three sub-groups:

- Empirical models (like Lucas-Tooth/Price or extended Compton)
- Fundamental parameter models (FPM)
- Specials like Layer Thickness

Fundamental parameter models calculate the inter-element effects on the basis of physical relations. In empirical models, all matrix effects have to be corrected on the basis of real measured standards.
One of the advantages of a fundamental calibration approach is the lower number of necessary standards (approximately one per element calibrated is recommended), but on the other hand the demands on the standards for an FPM are higher. As all inter-element influences are calculated on a theoretical basis the complete composition of a standard, even the concentrations of the elements not

measurable via XRF (i.e.: carbon, oxygen), are necessary.
Empirical models are commonly used for narrow ranges of matrix variation or if some other influences, like grain size effects, do not allow the use of fundamental parameter methods.

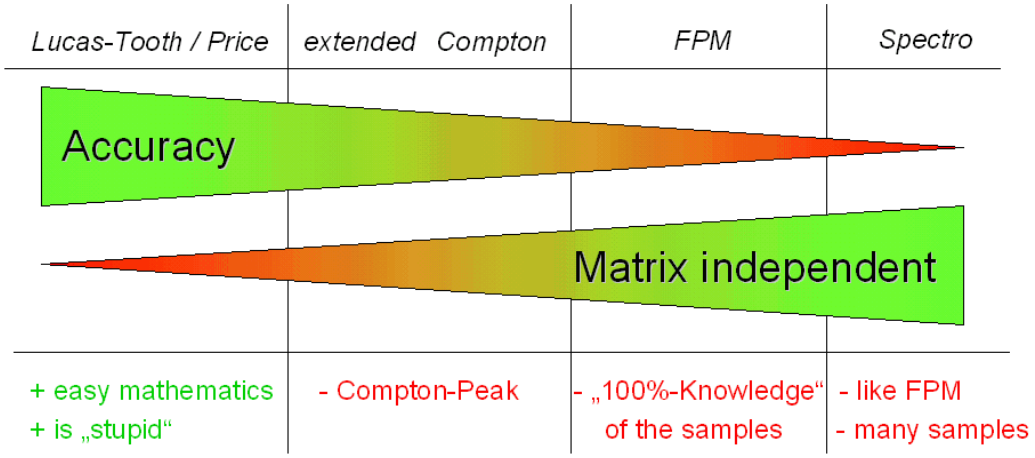
A brief description of the different models, their typical fields of application and some hindrances are listed in the following table:

Calibration Model	Typical Application
Lucas-Tooth, Price	Analysis of low-Z elements (Na to Fe) as main and minor elements. Especially in slag, dusts and minerals when particle size effects hinder a theoretical calculation.
Standard based FP (thick)	Main, minor and trace elements in a varying but known matrix, i.e. additives in oil.
Standardless FP (thick)	As FPM (thick): The normalization to 100% is only useful, if all main and minor elements can be analyzed, i.e. alloys.
Standard based FP (thin)	Low sample amount on filter material (i.e. aerosols), very thin films.
Standardless FP (thin)	As FPM (thin): The normalization to 100% is useful, if all of the main and minor elements can be analyzed. Typical application is the rubber technique with diamond paper. The method works without calibration.
Layer thickness model	Analysis of the layer thickness on a substrate, i.e. Aluminium on Silicon wafer.

In addition to the calibration models above, some general options can be set here. The calibration models will be explained in the following in more detail.

The following figure compares the four most common procedures with their advantages and disadvantages:

Comparison of calibration procedures



This figure compares the four procedures regarding *Accuracy* and how much they are *matrix indepentent*. The meaning of this comparison is that Lucas-Tooth/Price is the procedure using a minimum of mathematics which results in the best accuracy. The more mathematics are used, the bigger the deviations.
On the other hand, the models located at the left side of this figure, are not able to handle different matrices or a wide range of concentrations in the same calibration. If it is important to use a method, which is matrix independent, one of the models of the right side of the figure should be used.
But then there can be a bigger deviation between expected and calculated results:

In addition, there are some individual advantages / disadvantages for each procedure:

- Lucas-Tooth/Price: The advantage is the simple algorithm. It can be controlled using a pocket calculator and it is "stupid", that means, there are no physical / logical tests (e.g. a concentration can be > 100%) - this can be used for special jobs
- Extended Compton: The most important limitation for this model is the Compton-peak, which is needed. If in measurement no sub-measurement using a Compton-Target is defined, this procedure cannot be used for calculations.
- Fundamental Parameter Model: Defining the given concentrations, the software has to know all information about the elements in the calibration standards, e.g. if a Diesel, containing 400 ppm of Sulphur should be defined, the residual nearly 100 % of "oil" are important for the procedure, too. This 100%-knowledge can be a big problem.
- Spectro-procedure: Disadvantages are the same as for FPM, additionally more samples (especially for mac) are needed.

Unfortunately it is not possible to give a general answer to the question, which procedure should be used. There are too many details influencing this decision e.g. elements in the samples, concentration range...

One possible way is, to start with the easiest (especially mathemetics) procedure to get an impression about the correlation between intensities amd concentration. If Lucas-Tooth/Price is able to solve this application problem, it's the best choice. If it is not able to solve it, the next procedure can be tried (Ext. Compton, if a Compton-Peak is available).
The physical procedures using a lot of mathematics inside should be used at last or if completely unknown samples should be analyzed.

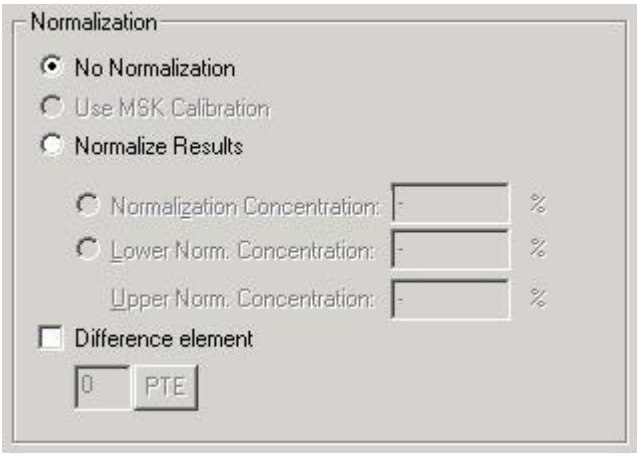
Matrix for Calib. (Element Bonds)

If this option is selected, all elements will be converted to their bonds. This makes it possible to calculate concentrations for low-Z elements (especially Oxygen) without measuring them directly. These calculated values for the low-Z elements will be taken into account during matrix correction.

If Matrix for Calib. should be used, they can be selected in General from a set of predefined bonds. To edit / create predefined *Bonds* the Configuration Editor has to be used.

Normalization

All options for the normalization are concentrated in the *Normailization* region on *General*.
The normalization procedure allows to force the sum of the concentrations on a specific value (defined by *Normalization Concentration*). This function influences the concentrations after the calibration. The options *MSK* (mac) and *Normalization* to a fixed concentration are not possible at the same time. When *MSK* is selected, an additional tab is displayed in the *calibration* tab.
The use of a *Difference element* is an additional option. This can only be one of the non-visible elements (typical H to F). If this option is used the difference between the sum of all analyzed elements and 100% is calculated as the difference element. It is possible to select bonds for the difference elements (see sub-method *evaluation*) to define matrices like $(CH2)_n$ for an organic sample.



The option *Normalize Results* normalizes the results before each iteration step, so that the matrix effects are calculated again based on the new information. The option *Normalize Results* will be performed after the last iteration. This will always lead to a sum of all concentrations equal to the *Normalization Concentration*.
These options can be used successfully, if all elements can be analyzed directly (i.e. alloys) or if the bonding state of the elements is exactly known (i.e. oxides in fusions) and the option *Matrix for Calib.* is selected at the same time.

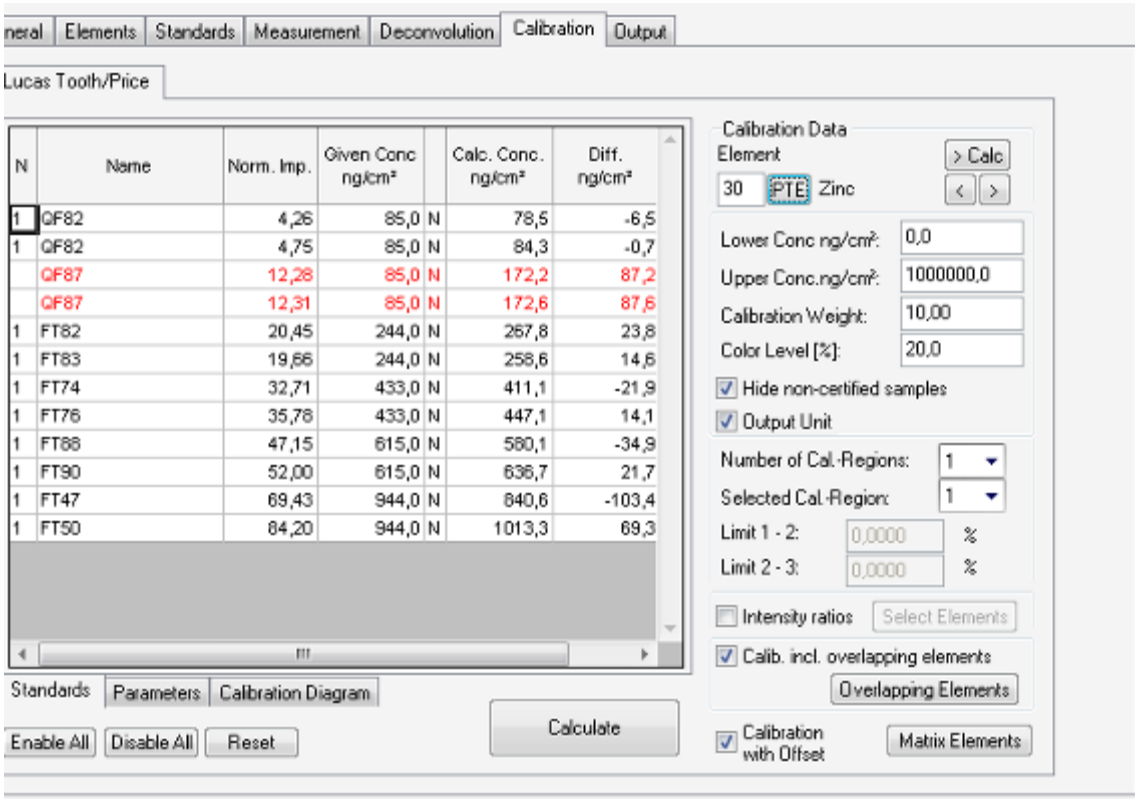
This normalization has nothing in common with the normalization on the Compton scattering peak or the normalization on regions of spectra used in the evaluation process.

30.2 Empirical Calibration using Lucas-Tooth/Price

The easiest possible correlation between intensity and concentration is the following:

*concentration = calib-factor * intensity*.

This describes the procedure called **Lucas-Tooth/Price**.
In detail we find a lot of possible corrections like Offset or 2 types of Interelement-Corrections (Overlapping elements and Matrix elements).



This card shows on the left side the list of the **standard samples**.
There are two possible presentations: If the option *"Hide non-certified samples"* (at the right side) is enabled,
two important conditions will control, if a sample appears in this list:
The standard needs a given concentration for this element AND intensity is found for this element during evaluation.
If this option is disabled, one of these conditions is enough, because it is an OR-condition.

This *standard list* contains different columns:

N	This column shows, if the sample is a part of the calibration and about its weight: **None** Sample is not in the calibration **1-5**

	The sample is in the calibration. The number shows, how many times this sample will be in the calibration
Name	That's the name of the sample
Norm. Int	The normalized intensity of the selected element in this sample. We like to use normalized intensities, because using them, we are able to handle different tube currents and/or measurement times in the same calibration.
Given Conc.	That's the goal
C	The certification level describes, how "sure" the given concentrations are: **N** Not analyzed. simple: not analyzed **L** Laboratory The given concentration is measured using another instrument **I** Info At a certification paper some values are certified as "Info" **C** Certified The given concentration is certified
Calc. Conc.	The result of the calibration
Diff.	To check the quality of the calibration, the differences between calculated and given concentrations are an important number.

At the right side of this sample list, some options were located, explained in the following:

Lower Conc./Upper Conc.:
These two values were calculated by the calibration mathematics - please do not change them

Calibration Weight

That's a value to control the calibration range, which should be important. If the calibration for smaller concentrations should be increased, reduce the value and vice versa for high concentrations...

Color Level

After the calibration is done the sample are shown using black or red color: The red color means, that the difference between given concentration and calculated value for this sample is too big. The limit, if a line is printed red or black, is this parameter (in % relative).

Hide non-certified samples

This option controls, which samples are shown in the sample list.

Output Unit

The concentrations in the standard list are presented in the internal unit "ppm". Most times it is more comfortable to use the unit, which is used for the printout.

Calibration regions

Only for Lucas-Tooth/Price it is possible, to calibrate using up to 3 regions. If more then 1 region is selected, the limits to switch between the regions have to be defined. The presentation on this card shows only the selected region. As result, the region which is interesting has to be selected. All following steps are now for this region. If another region should be modified, it has to be selected first..

Possible Corrections:

Intensity Ratios

That's an **unusual correction** option, only available for this empirical model (Lucas-Tooth/Price): These are normalized matrix elements (normalization of count rates or weighting of the concentrations). This leads to better analyzes of samples with irregular surfaces. When using this correction, the calibration should be checked with a large number of samples

Overlapping Elements

Elements that influence the deconvolution of the main line of the element of interest through peak overlap. If systematic error occurs (because of this) during deconvolution, the respective elements should be selected here. For example the K-lines of S are overlapped by the M-lines of Pb. This overlapping can lead to a systematic error. Pb should be entered as an overlapping element for S.

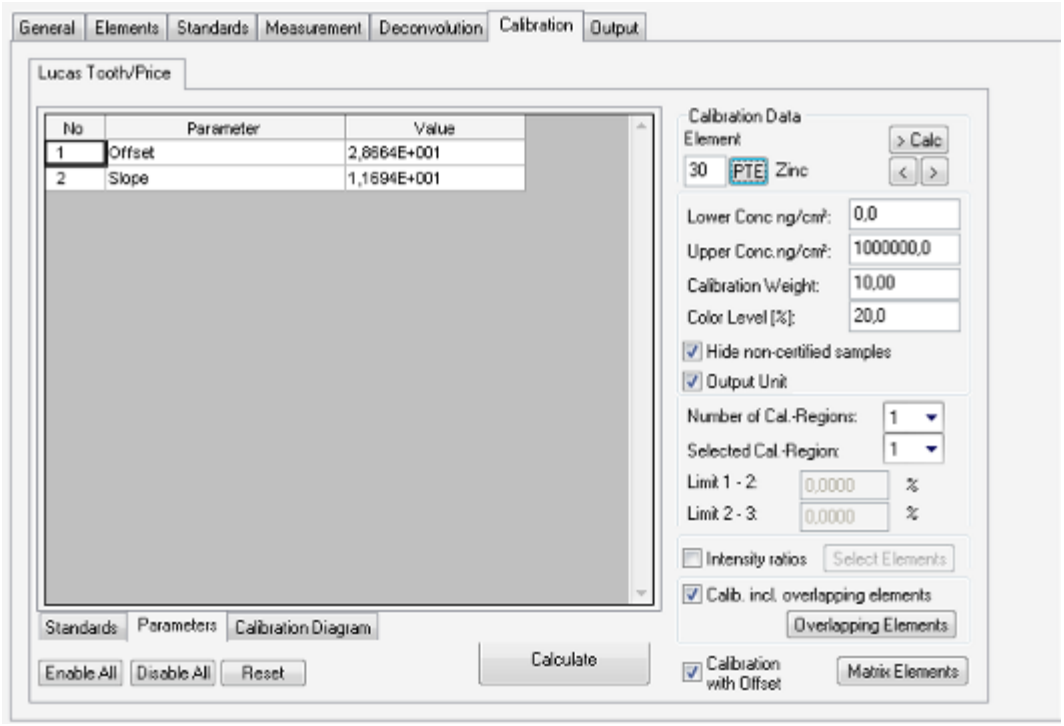
Matrix Elements

Secondary excitation and discontinuity elements are entered as matrix elements for the Compton model. Secondary excitation elements are used for Fundamental Parameter Models. Elements that have a matrix influence on the element of interest are entered for Lucas-Tooth/Price

Offset

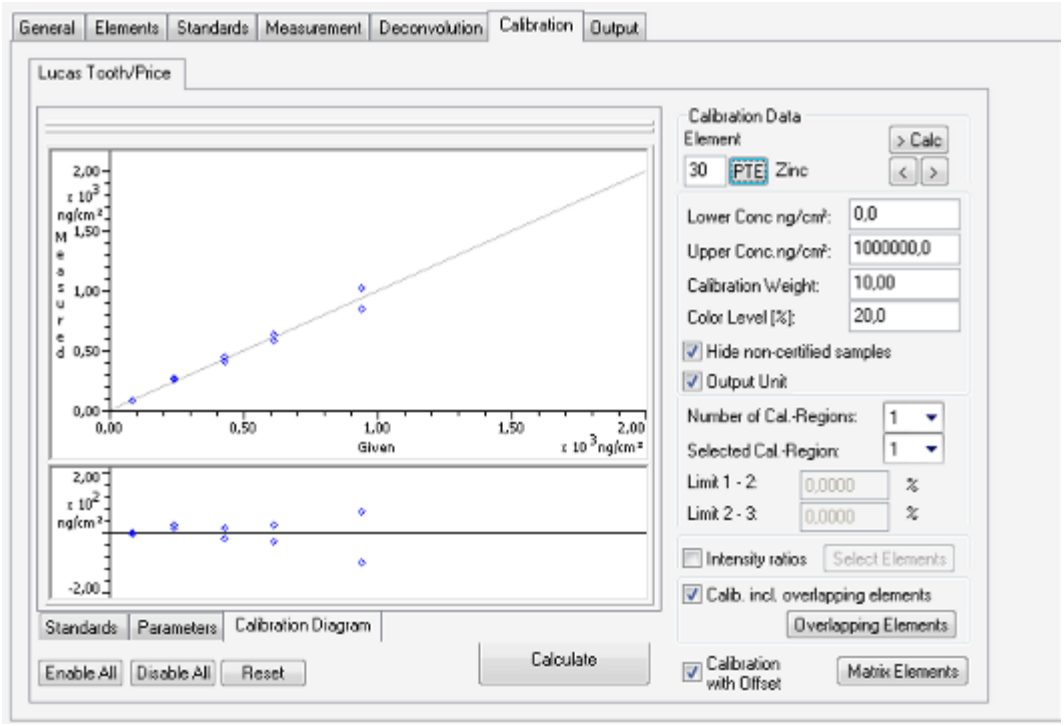
If the calibration needs an offset, this can be enabled here.

Parameters:



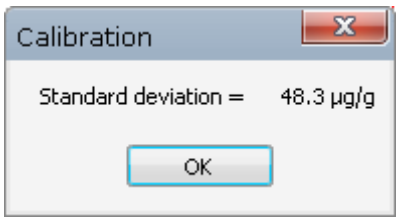
The card Parameters shows the calibration parameters.
After a successful calibration the Slope should be shown. All other parameters are additional options.

Calibration Diagram:



The Calibration Diagram shows the calibration line. The different signs are showing the level of certification.
If the right mouse button is used, a context menu is available, to select different options like linear or logarithmic scaling.
Touching a sample with the mouse, an info-box appears, that shows some details regarding this sample.
A double-click in the top-line (with the double-line) opens the diagram as full-screen version.

Calculate:



The button Calculate will start the mathematical procedure to calibrate the selected element. If no errors occur, this ends in the window which informs about the standard deviation during the calibration.

Enable All/Disable All:

A faster way - especially if a complete new method has to be calibrated and each sample is disabled - to enable samples for calibration is the "all"-feature. Instead of marking each sample individually by clicking, it is much more comfortable to select all samples using this feature.

Reset:

This function allows to reset the calibration to the last set of parameters, if the actual calibration was not successful.

Print:

It is possible to print the calibration data (samples, results, parameters, standard deviation) e.g. for documentation.

If something is going wrong or if some unexpected results were calculated, an error message will appear, which informs about the problem.

30.3 Calibration based on a Fundamental Parameter Model (FPM)

There are two different types of calibrations built-in in X-Lab^{Pro}:

EMPIRICAL CALIBRATIONS and FUNDAMENTAL PARAMETER MODELS

The empirical procedures like extended Compton or Lucas-Tooth / Price try to find a correlation between intensities and concentrations using "stupid" mathematics - if the calculated parameters can be explained or not.

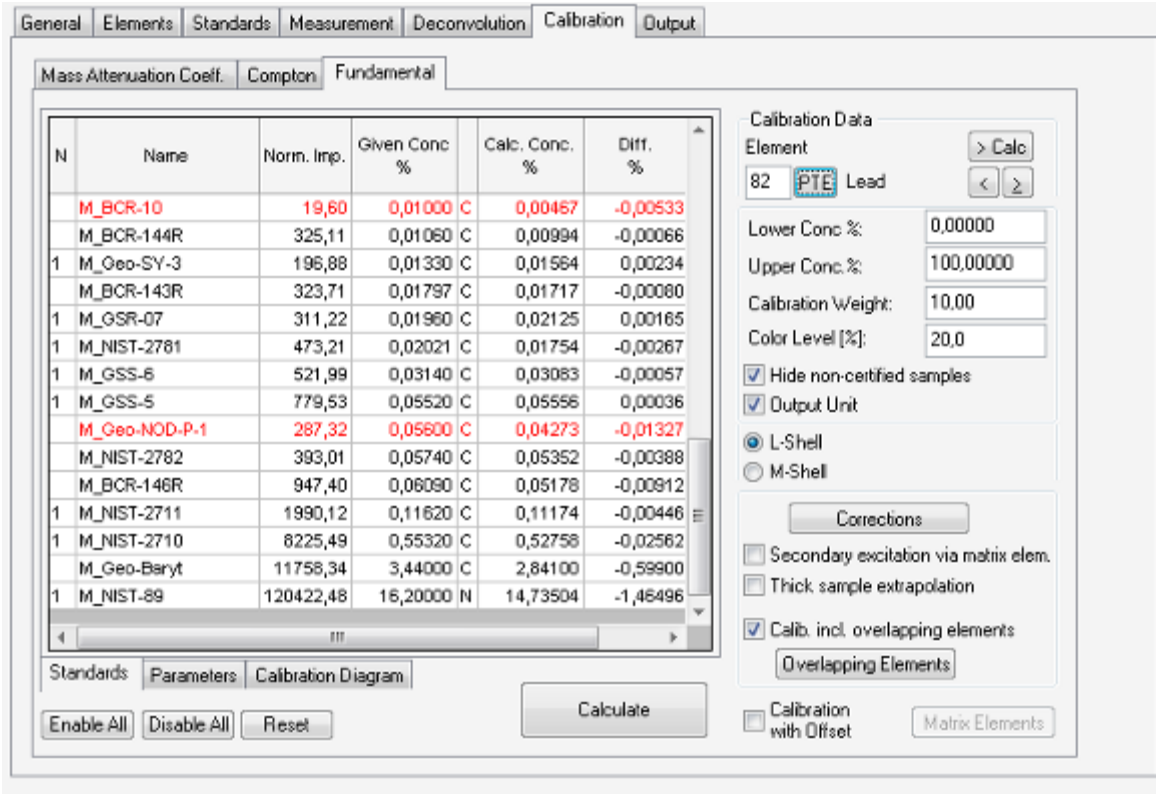
The complete opposite of this strategy are ***Fundamental Parameter Models.*** They try to explain the sample during the calibration and the evaluation of unknown samples. It's not just a calibration factor together with an intensity which is creating the result - it's much more...

During the calibration all known information about the sample is taken into account. These are much more then the given concentration. These are in addition all other concentrations (including "non-visible" elements like Oxygen), Loss of ignition, the (theoretical) Mass Attenuation coefficient based on the concentrations....

All this together is used for calibration. If the calibration is done and unknown samples are analyzed the evaluation is again not easy, because all calculated information/concentration are used to calculate the element of interest. Unfortunately the concentration of this element can have an influence to other elements.
As result the calculation of the other elements has to be repeated, which will influence again the element of interest....That's a big circle and at the end we will find some concentrations.

The calculated concentrations are responsible for the spectra - that's the theory of the FP-Model.

Following the calibration screen for Fundamental Parameter Model is described. This description takes care for the differences to Lucas-Tooth / Price. Similar functions are explained there.



K-Shell/L-Shell:

That can be an option for future...not available yet.

Secondary excitation via Matrix Elem.:

This option allows to work with Matrix Elements, which can be defined, using the "Matrix Elements" icon.

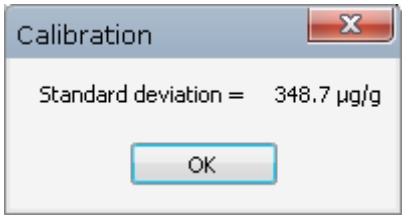
Thick sample extrapolation:

For light elements a sample with a thickness of several millimeters is thick compared to the penetration depth.
But the heavier the elements, the bigger the penetration depth of the exciting radiation.
For heavy elements the thickness of the sample influences the intensity in the spectrum.

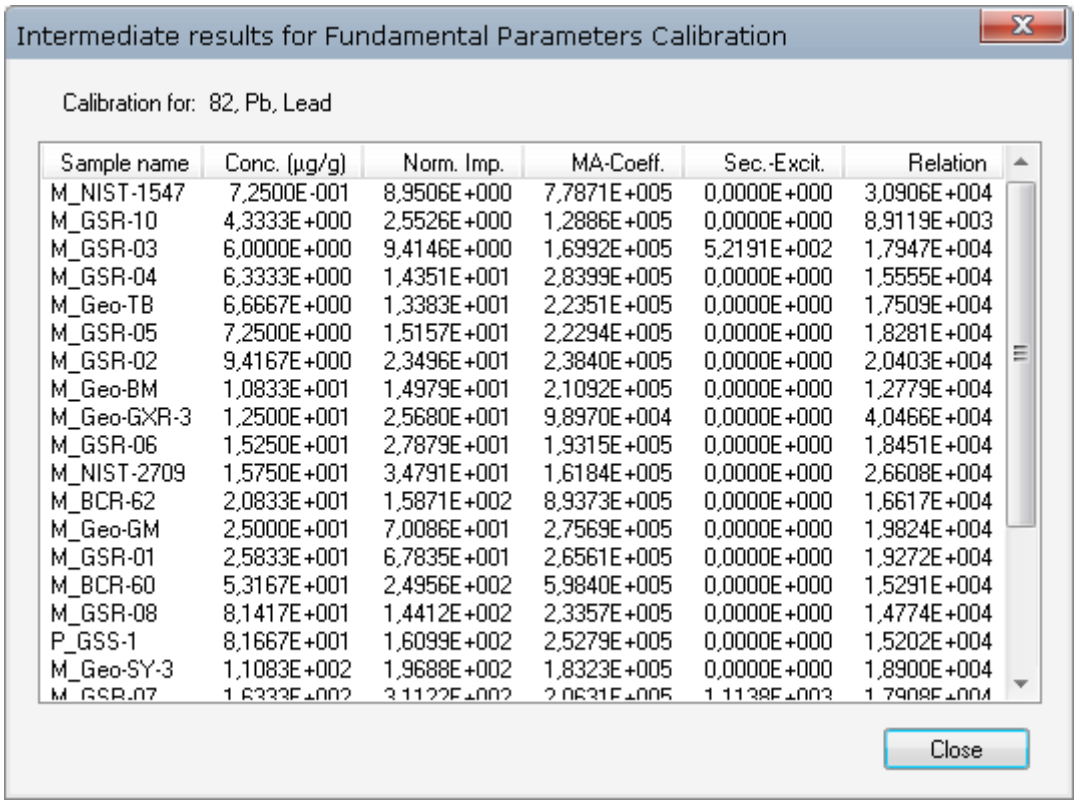
This parameter uses the sample thickness for calculations. Depending on experience and physical data, this parameter is used starting at Bromine (Br = 35).

Calculate:

after pressing calculate, the calibration is done, but before the final window shows the standard deviation



an additional screen presents some intermediate results:



Sample name	Conc. (µg/g)	Norm. Imp.	MA-Coeff.	Sec.-Excit.	Relation
M_NIST-1547	7,2500E-001	8,9506E+000	7,7871E+005	0,0000E+000	3,0906E+004
M_GSR-10	4,3333E+000	2,5526E+000	1,2886E+005	0,0000E+000	8,9119E+003
M_GSR-03	6,0000E+000	9,4146E+000	1,6992E+005	5,2191E+002	1,7947E+004
M_GSR-04	6,3333E+000	1,4351E+001	2,8399E+005	0,0000E+000	1,5555E+004
M_Geo-TB	6,6667E+000	1,3383E+001	2,2351E+005	0,0000E+000	1,7509E+004
M_GSR-05	7,2500E+000	1,5157E+001	2,2294E+005	0,0000E+000	1,8281E+004
M_GSR-02	9,4167E+000	2,3496E+001	2,3840E+005	0,0000E+000	2,0403E+004
M_Geo-BM	1,0833E+001	1,4979E+001	2,1092E+005	0,0000E+000	1,2779E+004
M_Geo-GXR-3	1,2500E+001	2,5680E+001	9,8970E+004	0,0000E+000	4,0466E+004
M_GSR-06	1,5250E+001	2,7879E+001	1,9315E+005	0,0000E+000	1,8451E+004
M_NIST-2709	1,5750E+001	3,4791E+001	1,6184E+005	0,0000E+000	2,6608E+004
M_BCR-62	2,0833E+001	1,5871E+002	8,9373E+005	0,0000E+000	1,6617E+004
M_Geo-GM	2,5000E+001	7,0086E+001	2,7569E+005	0,0000E+000	1,9824E+004
M_GSR-01	2,5833E+001	6,7835E+001	2,6561E+005	0,0000E+000	1,9272E+004
M_BCR-60	5,3167E+001	2,4956E+002	5,9840E+005	0,0000E+000	1,5291E+004
M_GSR-08	8,1417E+001	1,4412E+002	2,3357E+005	0,0000E+000	1,4774E+004
P_GSS-1	8,1667E+001	1,6099E+002	2,5279E+005	0,0000E+000	1,5202E+004
M_Geo-SY-3	1,1083E+002	1,9688E+002	1,8323E+005	0,0000E+000	1,8900E+004
M_GSR-07	1,6333E+002	3,1122E+002	2,0631E+005	1,1138E+003	1,7908E+004

If something has gone wrong or if some unexpected results are calculated, an error message appears, which informs about the problem.

Corrections:

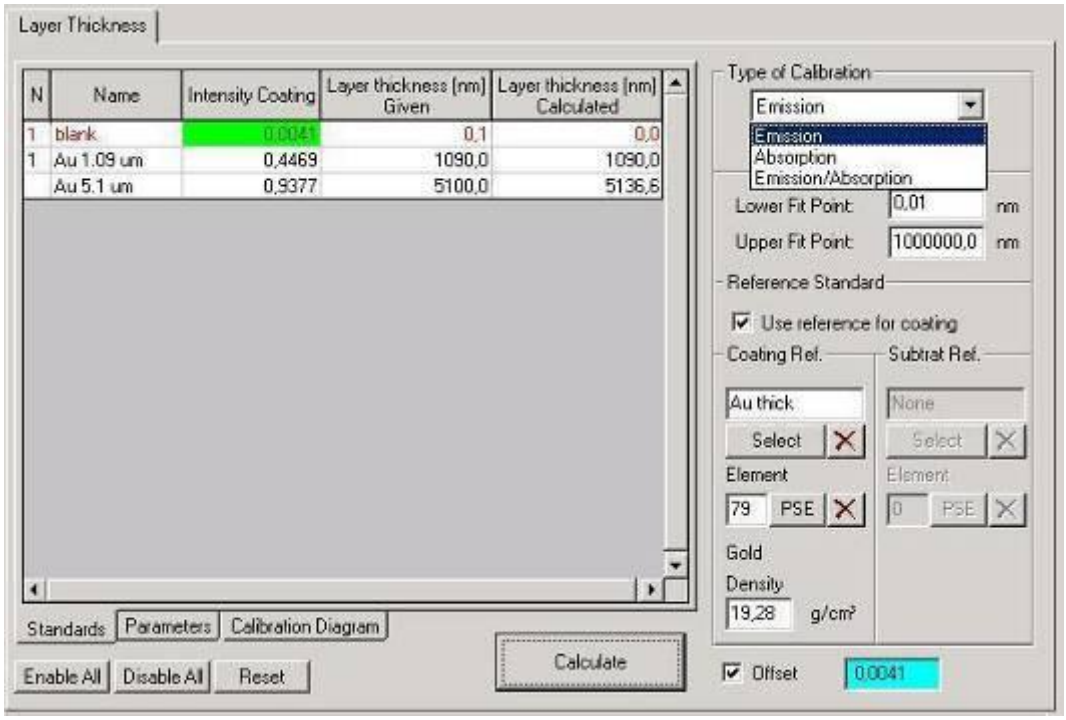
There are three places to select corrections at this calibration screen:

- Overlapping Elements
- Matrix Elements
- Calibration with Offset

30.4 Special procedure for Calibration of Layer thickness

Analysis of the layer thickness on a substrate, e.g. Aluminum on Silicon wafer or layers of Gold.

The card looks different compared to the other procedures, because this calibration is a special one:



First of all a layer thickness can be detected in different ways:
- The **Emission** of the coating is detected and the thicker the coating is, the higher the intensity.
- The second way is **Absorption**: The observed intensity is created by the substrate.
  The thicker the coating is, the bigger the absorption of the radiation of the substrate and
  the smaller the intensity of the observed peak of the substrate element.
- The best way is a combination of both: **Emission/Absorption**

The first calibration can be used for Au-Layers on other metals, the second can be used, if the coating material is not visible for XRF (like plastic coatings) and the combination is used e.g. for wafers.

The example above shows case 1 (Emission of the coating material) for Gold layers. In this case some options for the substrate material are disabled, because the substrate is not taken into account.

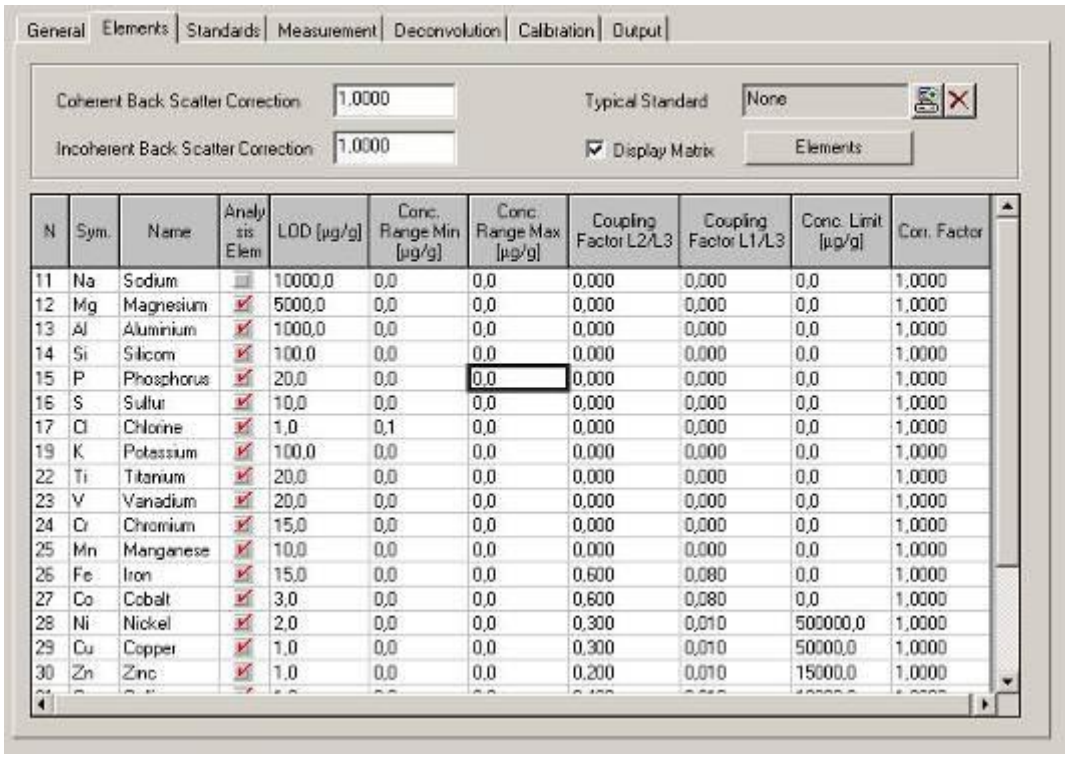
The calibration is completed, if the intensity, which is found for the blank sample (green high-lighted in the figure above), is used as "**Offset**" value (here: 0,0041) (light blue). **This has to be done manually !!!!**

30.5 Elements

This tab is one of the most important tabs in a method, because it contains a list of all elements, which

a) can be contained in the samples
b) should be analyzed.

Both will control the Measurement Conditions and the Deconvolution!



N	Sym.	Name	Analysis Elem	LOD [µg/g]	Conc. Range Min [µg/g]	Conc. Range Max [µg/g]	Coupling Factor L2/L3	Coupling Factor L1/L3	Conc. Limit [µg/g]	Corr. Factor
11	Na	Sodium	☐	10000,0	0,0	0,0	0,000	0,000	0,0	1,0000
12	Mg	Magnesium	☑	5000,0	0,0	0,0	0,000	0,000	0,0	1,0000
13	Al	Aluminium	☑	1000,0	0,0	0,0	0,000	0,000	0,0	1,0000
14	Si	Silicom	☑	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
15	P	Phosphorus	☑	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
16	S	Sulfur	☑	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
17	Cl	Chlorine	☑	1,0	0,1	0,0	0,000	0,000	0,0	1,0000
19	K	Potassium	☑	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
22	Ti	Titanium	☑	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
23	V	Vanadium	☑	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
24	Cr	Chromium	☑	15,0	0,0	0,0	0,000	0,000	0,0	1,0000
25	Mn	Manganese	☑	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
26	Fe	Iron	☑	15,0	0,0	0,0	0,600	0,080	0,0	1,0000
27	Co	Cobalt	☑	3,0	0,0	0,0	0,600	0,080	0,0	1,0000
28	Ni	Nickel	☑	2,0	0,0	0,0	0,300	0,010	500000,0	1,0000
29	Cu	Copper	☑	1,0	0,0	0,0	0,300	0,010	50000,0	1,0000
30	Zn	Zinc	☑	1,0	0,0	0,0	0,200	0,010	15000,0	1,0000

As first step (using the button *Elements* on top) all possible elements have to be defined.
These are the elements which can be in the samples.

All the selected elements are visible in the list, shown above.
Now, as second step, one can assign the elements of interest. This can be done by using the *Analysis Elem* column. If an element is marked here, the intensity of this element is fed to the calibration procedure to calculate a concentration.

The LODs are the Limits Of Detection for each element.

The column *Conc. Range Min. [µg/g]* defines the lower limit of the calibration and it describes the detection limit. The following column *Conc. Range Max. [µg/g]* is important to define the size of the concentration range.
That's an important information regarding the calibration procedure.
The values for both columns will be extracted from the method automatically.

Whether the columns called *Coupling Factor L...* and *Conc. Limit [µg/g]* are visible, depends on the user level.

The last column contains the correction factors, which are calculated during a Method Recalibration.
In addition to these factors the two factors for the scattering intensities (*Coherent Back Scatter Correction* and *Incoherent Back Scatter Correction*) are editable on top of the list.

If Bonds should be used, they can be selected from a set of pre-defined bonds at General and/or Output.
To edit / create pre-defined bonds the Configuration Editor has to be used.

30.6 Measurement

The setting of the measurement conditions is one of the first steps of the method development.
It is necessary to decide the purpose of the method first. Which are the critical parameters, detection limits or measuring time?
Is it possible to measure the samples in vacuum or is gas flushing necessary?
Which elements are important?

These questions have to be answered in advance to create a tailor made method for a specific application.

For almost all elements a variation of different excitation conditions exists for each instrument. The first step is to select the best target combination for a specific method.
A method is limited to 8 different targets. The number of targets used is influenced by the analytical needs and by the measuring time.

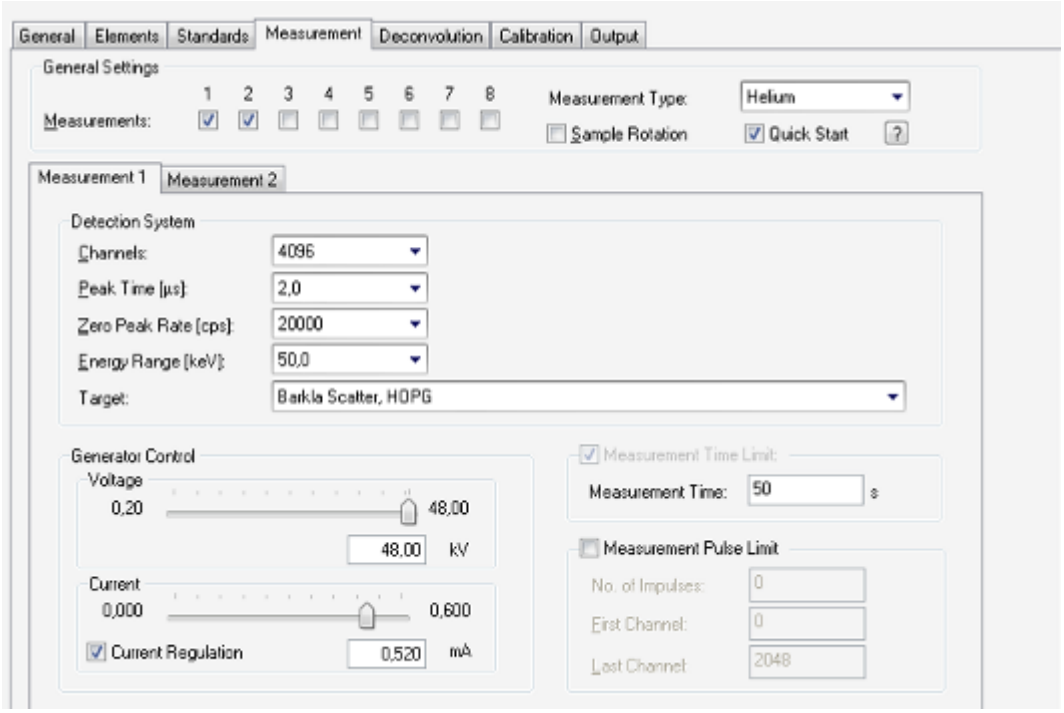
Some basic rules for the development of a measurement strategy:

1. Always start the method with the Compton target if you need the information of the Compton Scattering (for details: see Calibration).
2. Proceed with the target requiring the highest excitation energy. The information from this measurement about the concentration of the heavy elements can be used to improve the deconvolution of low-Z elements influenced by line overlaps of the L or M-Lines of the heavy elements.

Such a combination is Molybdenum and Sulfur: The Sulfur-K-line, which is used for calculations, is overlapped with the Mo-L-line.
Without any correction, Mo in the samples will influence the S-results. If the sub-measurement which calculates Mo-K is done before the S measurement the result of the latter can be corrected.

3. To analyze traces of light elements in a high-Z matrix, use a target that can only excite the analyte. This is only possible if the energy of the excitation source is between the absorption edges of analyte and matrix.
4. To increase the count rate, it is possible to increase the tube current. Increasing the tube current leads to a higher intensity of the radiation. Increasing the tube voltage not only changes the intensity, but also the spectral composition of the radiation. Thus, it is necessary to create new background spectra when the tube voltage is changed.

All measurement parameters are set in the sub-method *Measurement*.



The *General Settings* of the measurement are located in the upper half of the screen. The number of sub-measurements can be selected here. Additionally, the environmental conditions (vacuum, air or He-flush) are selected here.

The lower half of the screen contains the settings of sub-measurements for this method.

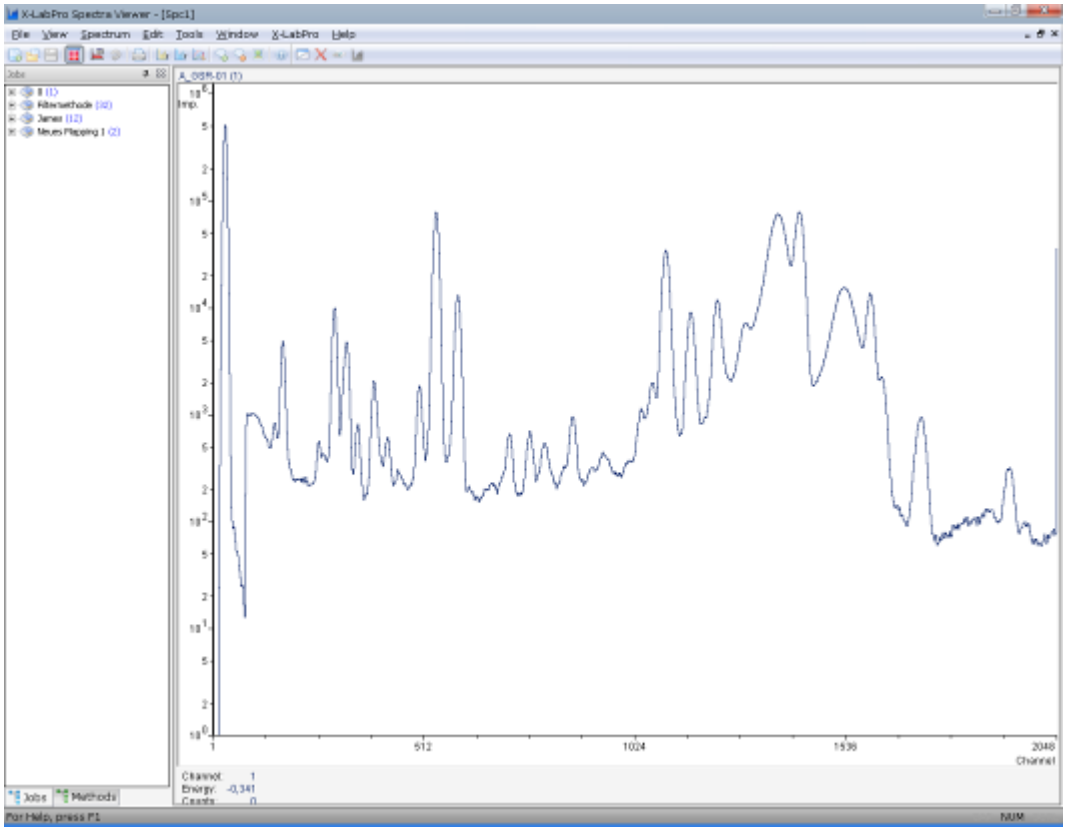
Some of the values in the lower part of the window should not be changed, others can be varied (see below). An overview of the parameters, the possible settings are listed in the table below.

Parameter	Notes
Channels	1024 and 2048 channels are recommended for measurements at the *Energy Range* 12,5 and 25 keV, respectively. For measurements at the *Energy Range* of 50 keV 4096 channels should be used. - **Do not change**
Peak Time [µs]	The time for the detection electronics to shape a peak. This time is a characteristic value for the detection electronics. It is important to note that all used combinations of *peak time* and *energy range* must be calibrated with the Method called MCA. - **Do not change**
Zero Peak Rate [cps]	Necessary for the accurate dead time correction - **Do not change**.
Energy range [keV]	The scaling of the x-axis of the spectra. For light elements we like to use 12.5 keV, for mid-range energies 25 keV and for heavy elements 50 keV. Each target or filter has its own recommended Energy range. - **Do not change**
Target	Selects the target for this sub-measurement.- **Do not change**
Voltage	The excitation depends on the voltage which is used. A voltage depending on the selected target/filter is recommended. Changes in the voltage will influence the background spectra which have to be modified after changing the voltage. - **Do not change**
Current	The optimum dead time is 25%. If *Current Regulation* in enabled (see next item), the current stored here is only the default start value. This will be regulated depending on the intensity which is influenced by the sample type.
Current Regulation	When this option is activated, the settings for tube current will be used as a starting current only. The software will measure the sample with the given settings and then optimize the tube current. The resulting intensity should not exceed 100,000 cps.
Measurement Time Limit	Default: This option is selected as standard stop criteria.
Measurement Time	This is the clock time for the measurement. It is not possible to select a live time. Live time = clock time * (1 - rel. dead time).
Measurement Pulse Limit	An alternative option to end a sub-measurement. If the number of counted impulses is bigger than the given value in *No. of Impulses* the measurement will stop. If both options (*Measurement Time Limit* and *Measurement Pulse Limit*) are selected, the criteria first met will stop the sub-measurement.
No. of Impulses	For the *Measurement Pulse Limit* option the criteria for stopping the sub-measurement can be set here.
First Channel	For the above listed option *No. of Impulses* the region of interest (ROI) must be defined. This is done with the two

	parameters *First Channel* and *Last Channel*. This is only necessary, if the option *Measurement Pulse* is used.
Last Channel	See above.

30.7 Spectra Viewer

The Spectra-Viewer is an important tool in X-Lab[Pro].



If elements should be identified using only the Spectra Viewer, please take care of the ARTEFACTS !

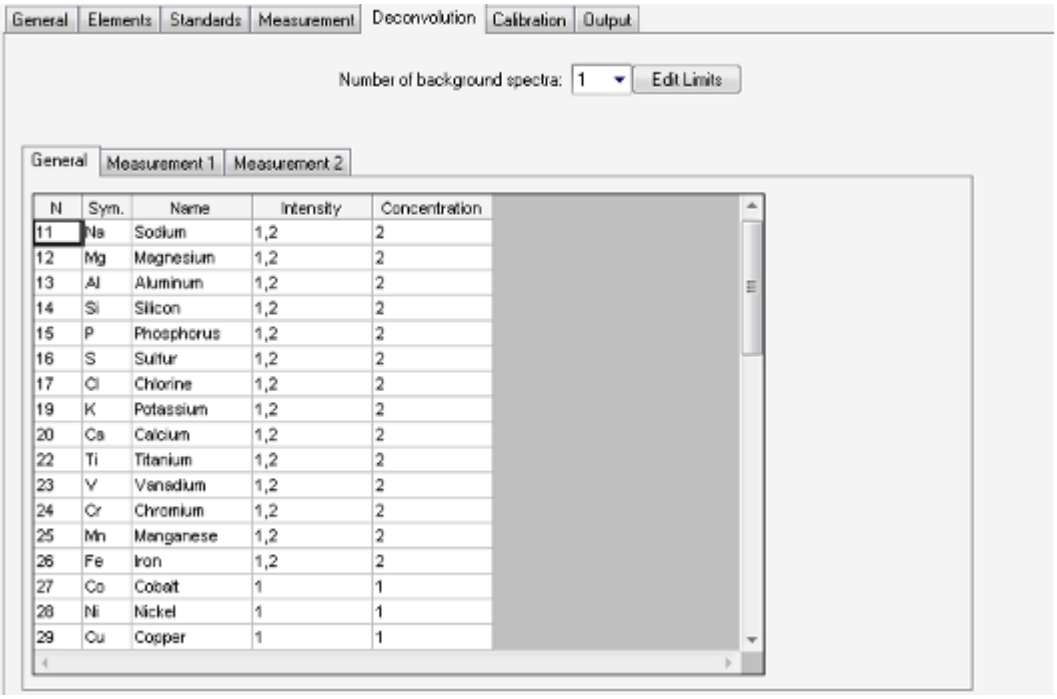
The Spectra Viewer can be used for method development, because the question, which elements could be in routine samples, can be answered a little bit easier using this tool.

This information is necessary to define the deconvolution together with the measurement conditions.

30.8 Deconvolution

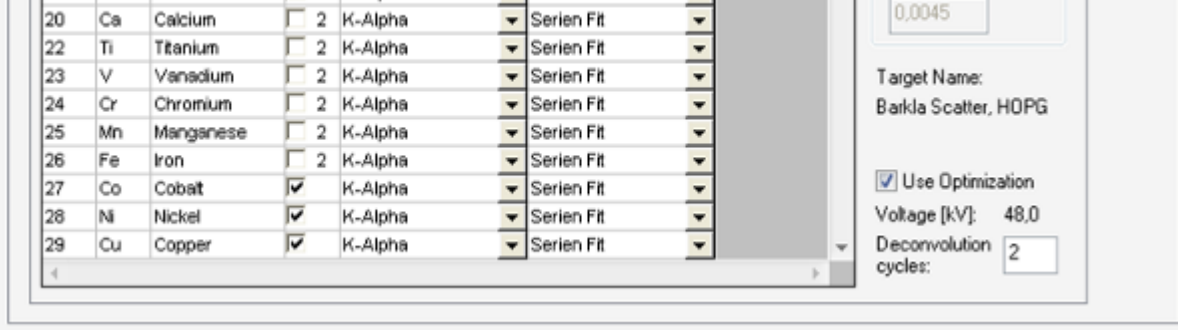
The deconvolution is necessary to determine the net counts for the individual elements of the method. This includes the subtraction of a background spectrum and a selection which lines should be used for the deconvolution. As a method is constructed of several sub-measurements, the parameters have to be defined for each of the sub-measurements. It is possible to deconvolute elements in several sub-measurements to correct for line overlaps, but it is only possible to calculate the concentration from a single sub-measurement.

The sub-method *Deconvolution* is divided into two kinds of tabs:
The tab *General* is a summary of the deconvolution to get an overview.



The number of background spectra and the corresponding switching limits can be selected here. The switchover values are the Compton to Rayleigh scattering ratios. Therefore, it is only possible to use several background spectra, if a Compton target is used in the method. With several background spectra available for each target it is possible to calibrate different matrices with a different scattered background (like organic and silicate samples) in one method.

The list shows, which elements have to be deconvoluted during evaluation in general. These elements can be selected at the tab Elements.
All elements which are present in a specific sample, should be selected. Even if the calculation of the concentration is not planned, it may be necessary to deconvolute the lines because of possible interferences and line overlaps.


20 Ca Calcium 2 K-Alpha Serien Fit
22 Ti Titanium 2 K-Alpha Serien Fit
23 V Vanadium 2 K-Alpha Serien Fit
24 Cr Chromium 2 K-Alpha Serien Fit
25 Mn Mangsnese 2 K-Alpha Serien Fit
26 Fe Iron 2 K-Alpha Serien Fit
27 Co Cobalt K-Alpha Serien Fit
28 Ni Nickel K-Alpha Serien Fit
29 Cu Copper K-Alpha Serien Fit
0,0045
Target Name:
Barkla Scatter, HOPG
Use Optimization
Voltage [kV]: 48,0
Deconvolution cycles: 2

The main part of the screen is a list of elements, which shows all selected elements, using the button Elements at the right side. The elements, which can be chosen at this place are pre-defined on the Elements tab. Only elements chosen on the tab are selectable here.

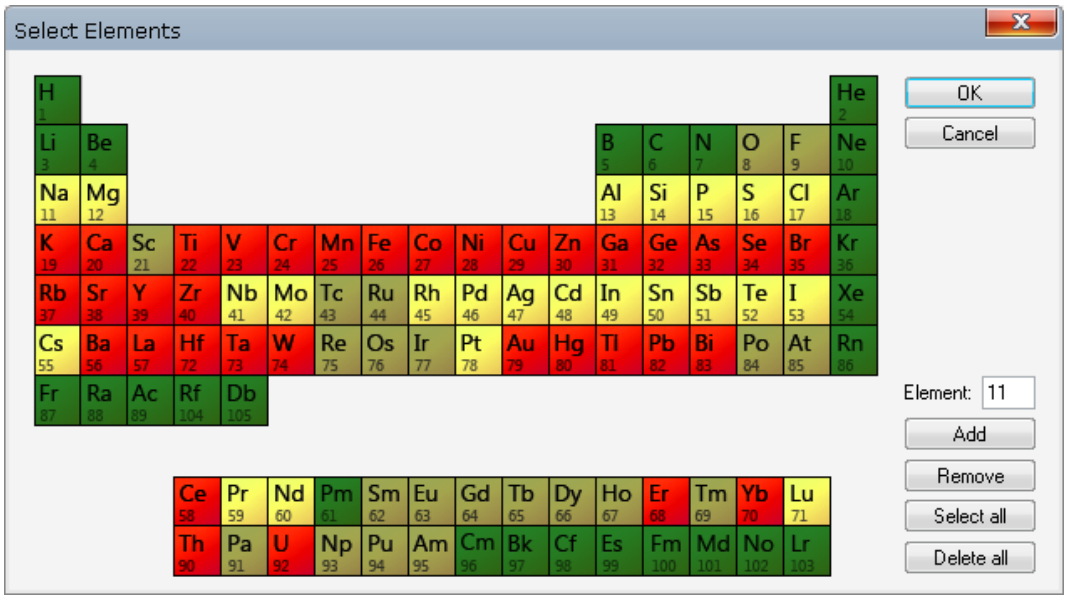
If an element appears in the list, the last three columns can be modified / defined:

The columns *Line* and *Deconvolution* describe the kind of calculation, which should be applied. For example, Sodium will be calculated from the K-Alpha line using *Serial Fit* as strategy. Possible strategies are:
- Summation,
- Series Fit ,
- Line Fit and
- Line Fit with Standardization

The check boxes in the column *Conc* are necessary to decide, whether an intensity is used for the calculation of the concentration or just as intensity e.g. for overlapping corrections. When a number is shown (like for Chromium) that means that the concentration for this element **must be** calculated using the intensity from a different sub measurement (Cr = 1).

On the right hand side there are 4 buttons to edit additional parameters.

Elements
If this button is selected a window with a periodic table of the elements will appear on the screen:



In this periodic table all elements that were selected in the tab Elements are marked in yellow and can be selected. All elements which can be excited in this

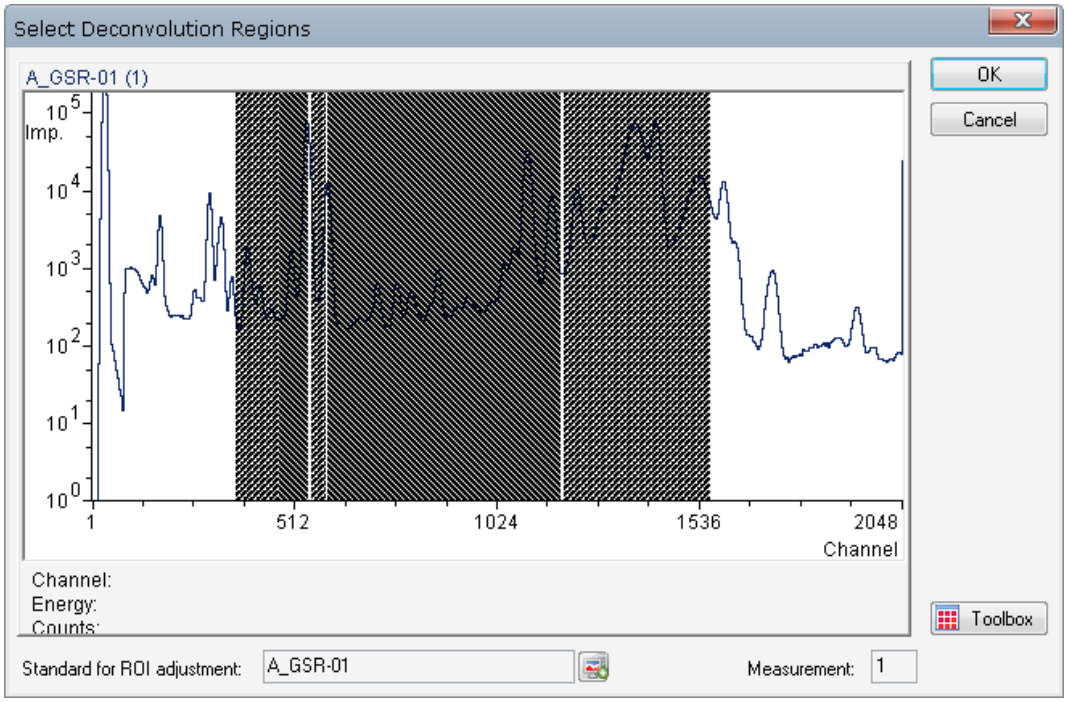
sub-measurement should be selected. To select an element, click the element symbol and the color changes to red.

All selected elements will be deconvoluted. It is not necessary to calibrate all of them or use them as concentration elements. For the Compton target it is essential to deconvolute the elements even if no concentration is calculated from the Compton target (like in most geological calibrations). In this way the overlaps with the scattering lines can be corrected.

Only the elements selected in this PTE can be ticked as "concentration elements" in column *Conc.*

Deconvolution Region:
Most of predefined SPECTRO methods do not require any changes in the deconvolution settings. If this is required for a specific application, the Optimization must be disabled

With the above defined settings all lines to be deconvoluted are selected, but it is not defined where the lines are and in which way they should be grouped in deconvolution areas. These deconvolution areas are selected with the button *Deconvolution Region*. These ROIs should be created in such a way that all elements are in ROIs but not too many lines in the same ROI.

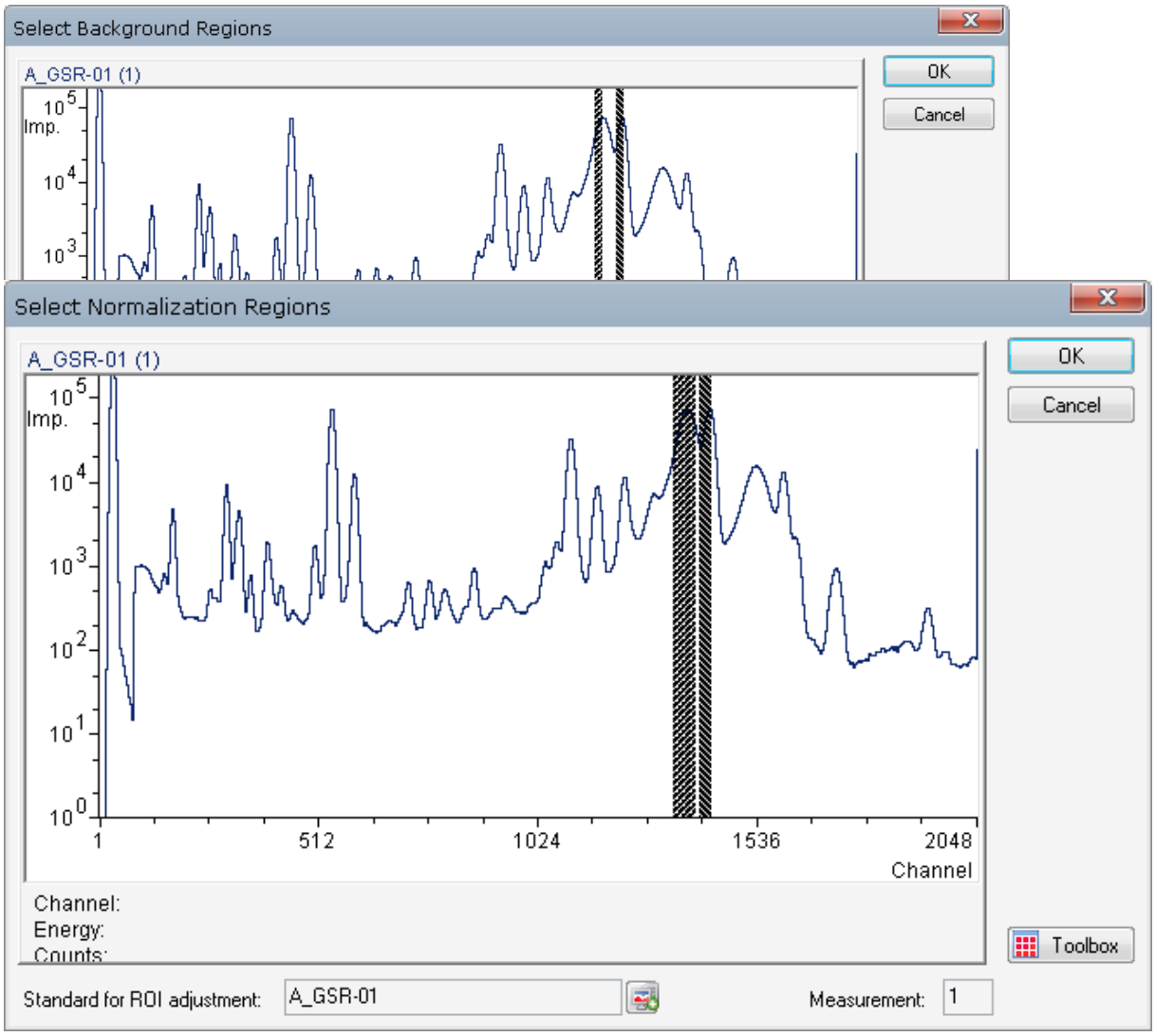


To create a ROI, the cursor is moved to the left edge of the planned ROI and then the right mouse button is pressed. When the mouse is moved to the right hand side – with still pressed mouse button – a region will be marked as ROI in a different hatching. To simplify the creation of the ROIs, it is quite useful to show the lines of the elements for this sub-measurement. This makes it easier to check, if all elements are in selected regions and if all lines of the elements with *Series Fit* are in the same deconvolution area.

To create the background regions, it is necessary to display a spectrum. The sample shown in the window can be selected at the bottom of this window. There's a list with all measured standards.

The deconvolution areas will be copied together with the rest of the parameters, when a method is copied. So, it is not necessary to edit all the regions.

Background Region:
A background spectrum can be fitted to the measured spectrum after some of the detector artefacts (as an example: pile-up, escape, shelf) have been corrected. To do this, fitting regions have to be defined, according to the way described under Deconvolution region:



These normalization regions can be used as an internal standard even for other sub-measurements. Two normalization regions are allowed per sub-measurement.

Iron-Cobalt-Correction:
With the button *Iron Cobalt Corr.* a special correction for Cobalt can be activated. This correction improves the determination of Cobalt traces in the presence of a

large amount of iron. The correction factor should not be changed. This special correction is only possible if the Co K_α and the Fe K_β- Lines are in separate ROIs.

Use Optimization:
By ticking the *Use Optimization* check box the parameters from the three buttons *Deconvolution Region*, *Background RegionNormalization Region* are calculated automatically.

The deconvolution of a sub measurement follows the rules:

The deconvolution areas (ROI, region of interest) are unfolded with increasing energy.

- In each ROI, the elements with *Line Fit* or *Line Fit with Standard* will be processed with increasing energy. The K_α-line (or the L_α-line) will be deconvoluted and founded on the net count rate.
- The additional lines of the same shell will be subtracted from the spectrum. For the L-series all lines of the three different sub-shells LI, LII and LIII will be considered. The coupling factors for the sub-shells can be edited in the *Evaluation* sub-method.
- Then all elements with a Series Fit are deconvoluted with increasing energy.

The deconvolution parameters are absolutely essential for the proper evaluation of a sub-measurement. Wrong or missing deconvolution parameters might result in severe problems of the software.

A *series fit* is only allowed, if all lines for one specific element are in the same deconvolution area (see Deconvolution Region) and if the background under the lines is not too different.
If the background is too different, the line ratio might be influenced and this will harm the accuracy of the *series fit*.

While copying a method all of the elements, lines and even deconvolution strategies will be pre-set, reducing the necessary effort to a minimum.

30.9 Deconvolution Strategies

The deconvolution is necessary to determine the net counts for the individual elements of the method.
This can be done, using different mathematical procedures:

- Summation,
- Series Fit,
- Line Fit and
- Line Fit with Standardization

The first one is used only for special applications (e.g. during a mapping using a MIDEX equipped with xyz stages).
To explain the differences between Line Fit and Series Fit, let's have a look, what happens with a new unknown sample during its evaluation:

The energy-range of a sub-method is divided in different Regions of Interest (ROIs).
These ROIs and their contents will be calculated from low-energy ROIs to high-energy ROIs.

Starting with the first ROI, the first step will be the **Line-Fit** for all Line-Fit-Elements:
It will start with the elements with the smallest Atomic-Number. In common cases the Alpha-line like K-Alpha is chosen. In this case, the K-Alpha-line of this element will be fitted. Based on this result, the corresponding Beta-line is calculated using a theoretical alpha-beta-ratio. After removing these lines (alpha and beta) from the spectra, the deconvolution will continue with the next element.
Doing this step-by-step (or element-by-element) all elements Line-Fit was chosen for, will be removed from the spectra.

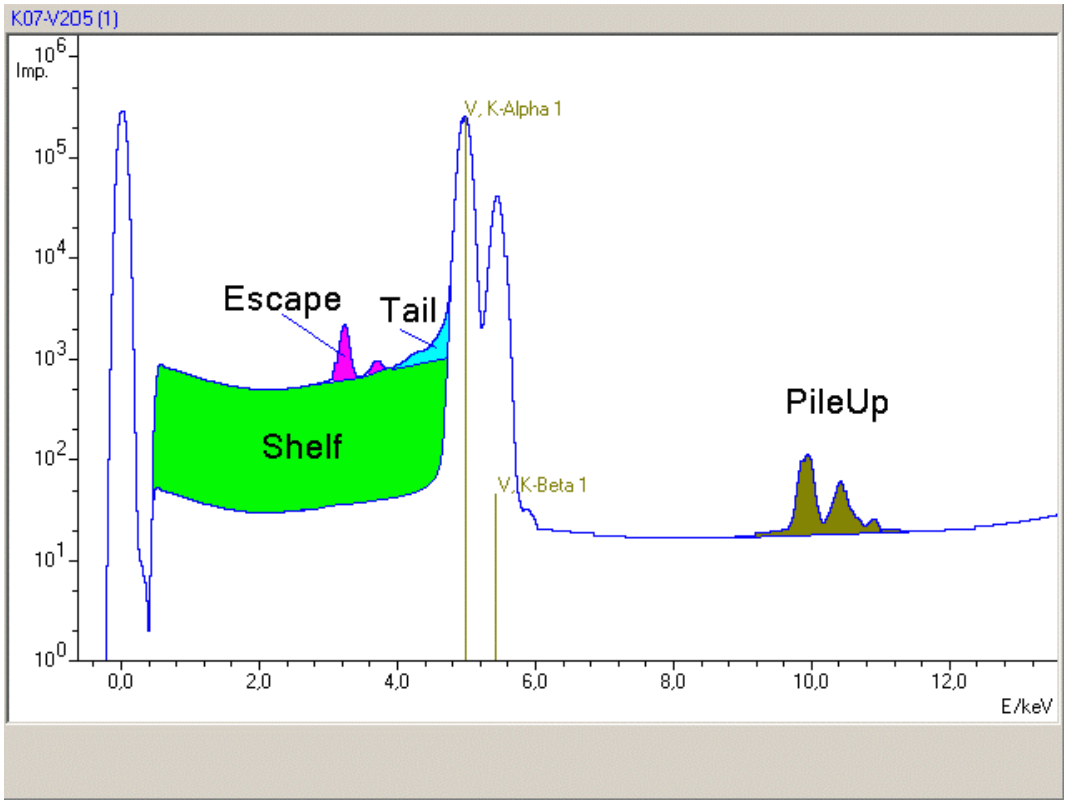
The residual spectra will be taken into a next deconvolution step:
In this last step, all elements with **Series Fit** (in one ROI) are deconvoluted in one step in a big equation-system.

Line-Fit with Standardization means that, if a minimum intensity is reached, the peak is used to recalibrate the energy-channel-calibration for this sample.

30.10 Artefacts:

The following figure shows a spectrum of the sample V2O5.
Without the artefacts the spectrum should contain the background information from the instrument and the V-lines.

But in reality the spectrum looks a little bit different than expected: In addition to the V-lines, it shows the 4 artefacts:
- Shelf
- Tail
- Escape
- PileUp



As the figure shows, SHELF and TAIL are both creating additional background at the low-energy side of a peak. Both decrease the S/N ratio with the result of increased detection limits.

If elements shall be identified manually, the artefacts described in the following are more difficult to handle, because they are creating "peaks":

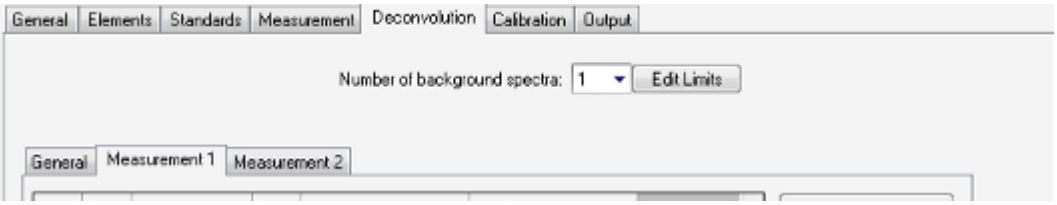
The artefact Escape has an energy which is reduced by around 1,75 keV compared to the "original"-peak. That's the energy of Silicon, which is used as detector chip material.

The PileUp occurs, when 2 photons, reaching the detector at the same time are identified as 1 photon with doubled energy. If the "original" peak is a single peak (because peaks cannot be separated) like Si-K-series, we will find 1 PileUp peak. The figure above shows what happens with 2 lines like alpha- and beta-line: These two lines will generate 3 PileUp lines, because 2 alpha-photons or two beta-photons or an alpha- with a beta-photon can combine.

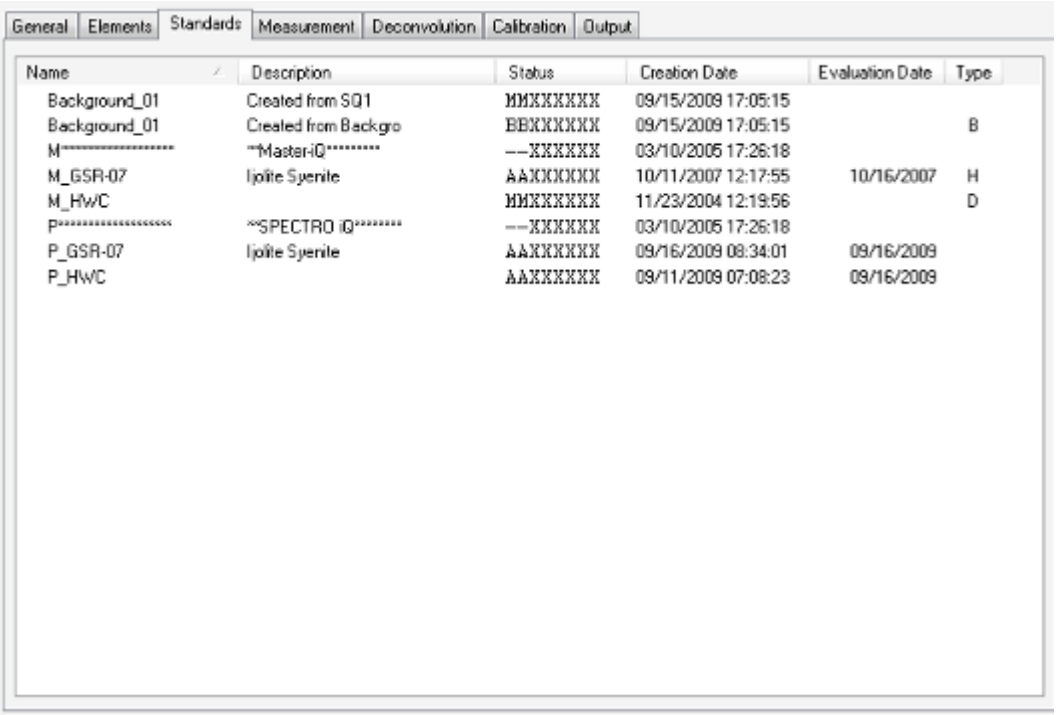
30.11 Background Spectra

One part of the evaluation of a measurement is the subtraction of the *Background Spectra*.

For each sub-measurement up to 6 Background Spectra can be stored (Deconvolution). In a SPECTRO iQ II only one background spectrum per method is typically defined.



The background spectra are stored as standards and at the Standards they are visible as it is marked with B.



It can be necessary to modify these background spectra depending on the application.

30.12 Background and Contaminations

In addition to the elements in the sample, which will have to be measured, there are some "contaminations" in the spectra, making the job a little bit more difficult.

"Contaminations" of Spectra:

****

The Target:
- HOPG-Target: The tube material (anode): Pd + Reflections

The Measuring Chamber:
- Iron

The Detector:
- Ta, Zr or Pd and a little bit of Sn (detector cooling)

All these "contaminations" together are visible in the Background spectra.

****

Sample Cups / Protection Film:
- Prolene: without contaminations
- Mylar: P and Ca
- Carbonat: Si

The Dilution Material:
- Oil: Sulfur
- Charcoal: a variety of elements

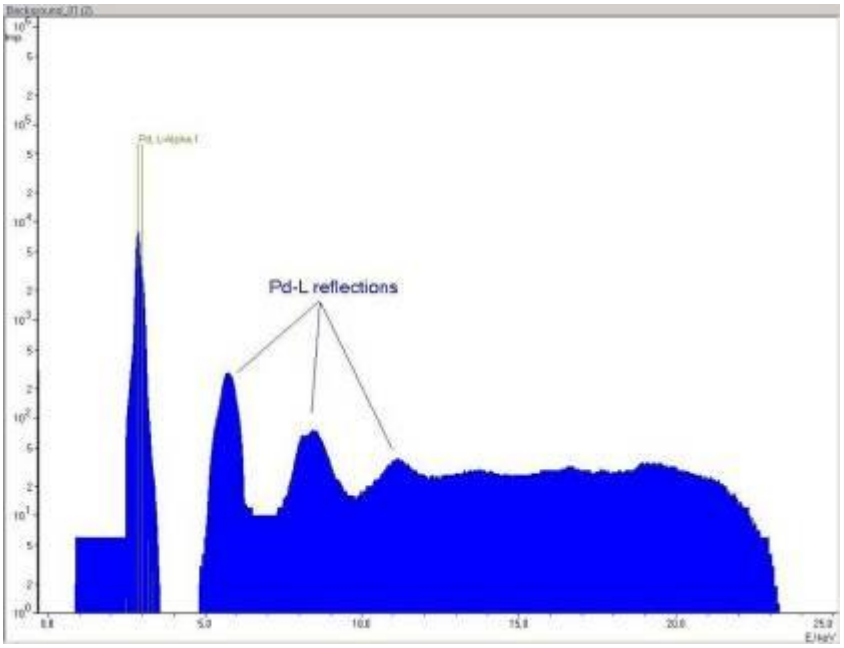
Artefacts

Contaminations in the instruments, e.g. after a foil crack, or caused by sample preparation

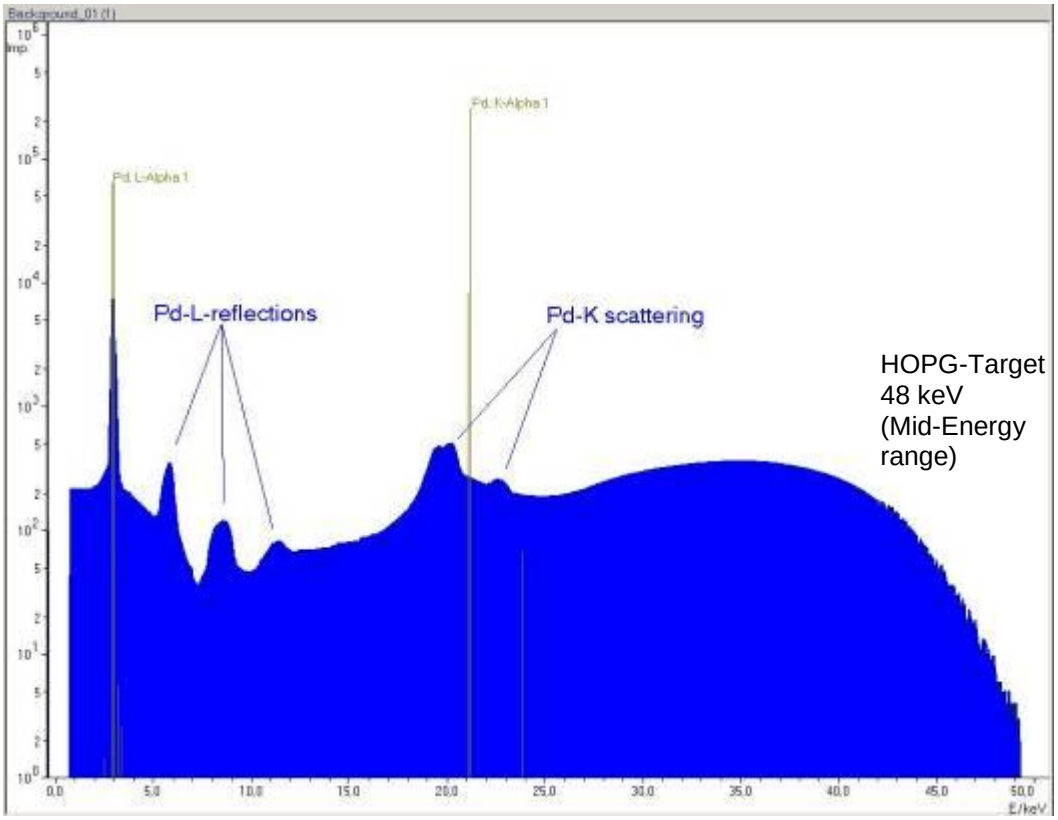
****

Background Spectra:

Background Spectra for SPECTRO iQ II:



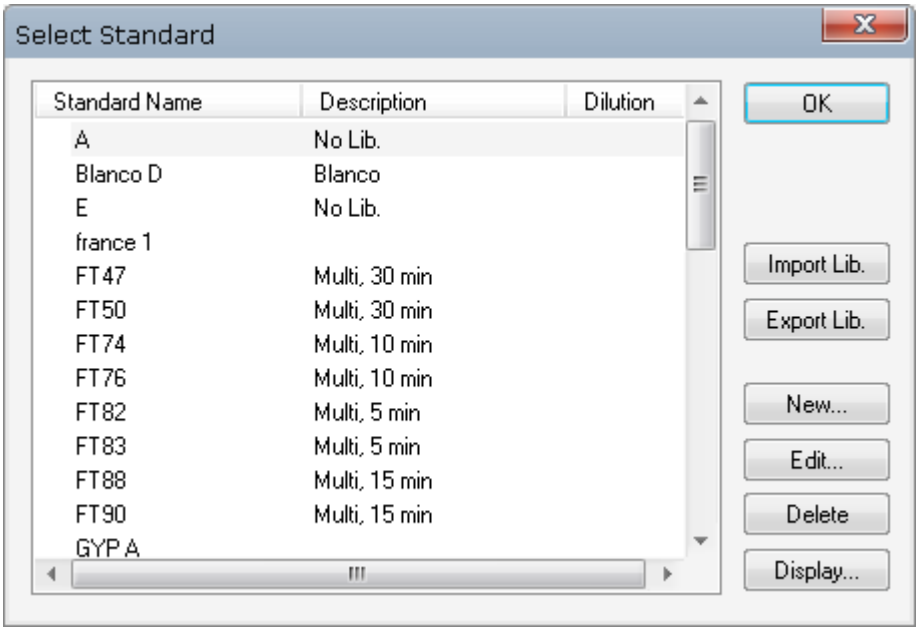
HOPG-Target 25 keV (Low-Energy range)



HOPG-Target 48 keV (Mid-Energy range)

30.13 Library of Standards

The Library of Standards is available in the menu *Tools*.



It is a database which contains the given concentrations of a lot of Certified Reference Materials (CRM). These data should be used during the creation of new samples used as standard:

It is much faster done, if the given concentration were copied/imported from this database instead of entering each element concentration.

30.14 Regions in Lucas-Tooth/Price

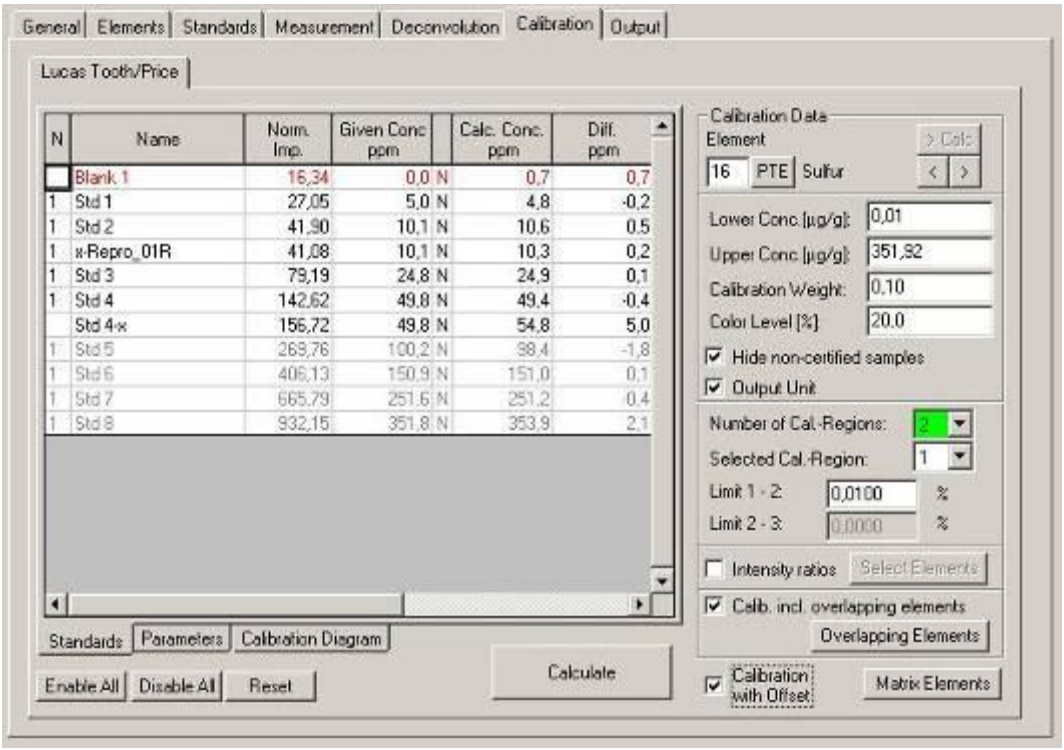
The Lucas-Tooth/Price calibration is the only one, which supports more then one calibration region.

This feature can be used, if the concentration range is too big to get good results.

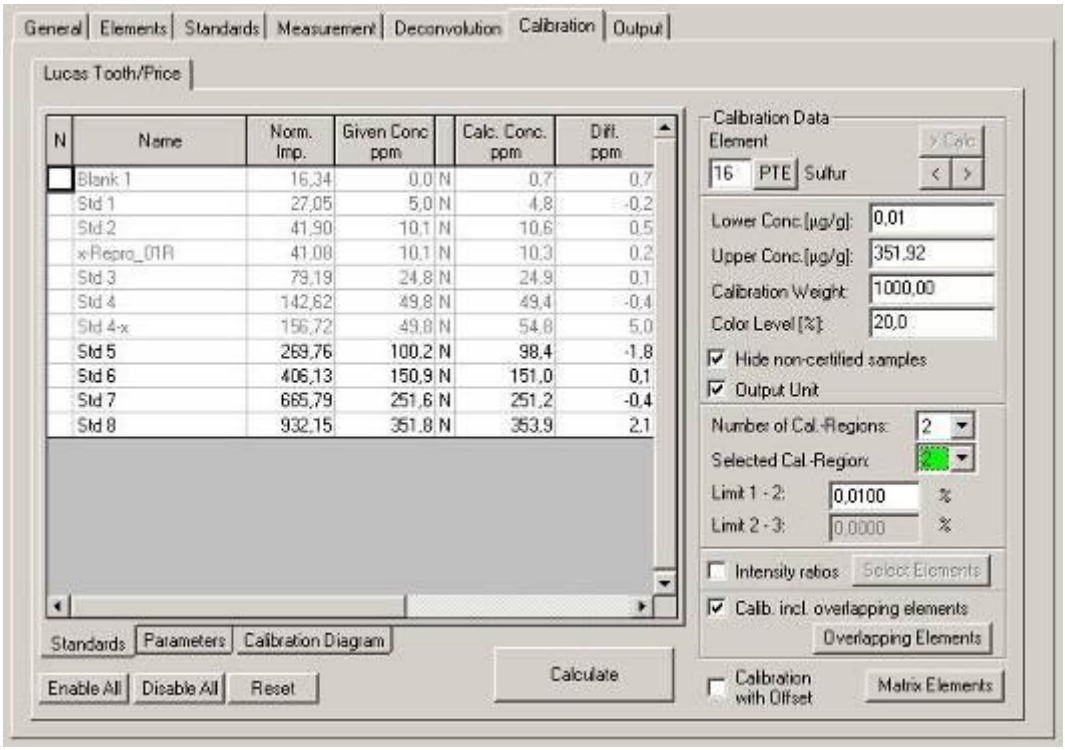
An example is Sulfur in Diesel. There are two possible regions:
- Around 400 ppm of S as common region and
- smaller then 10 ppm of S for Low-S-applications.

This example is used to show the region-feature.
First of all, the number of regions has to be increased. Doing this, the parameter "Limit 1 - 2:"
is used to define the switching-limit. That's the concentration, where the next region
(in this example region 2) starts. In the figure below, the limit is 10 ppm, that

means,
that for concentrations smaller then 10 ppm region number 1 is used and for higher concentrations region 2:

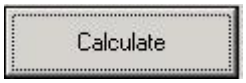


Pressing "Calculate" will calibrate only region 1!
The "Selected Cal.-Region:" shows, that the list at the left side is presenting the samples and results for region 1.
If the second region (> 10 ppm) should be calibrated, change the "**Selected Cal.-Region**" into "2":



After this change, pressing "Calculate" will calibrate the second region.

30.15 Error Messages during Calibration

After pressing 

some error messages can appear, if something unusual was calculated.

Following a summary of these messages:

Message	***Reason***	***Solution/next step***
Negative Offset	A negative Offset was calculated	**Remove** the Offset option
Offset seems to be too big	Offset is unexpected big	If the reason can be found and explained, the message can be ignored (1)
Incorrect correction	The calculated correction cannot be explained by Physical laws	**Remove** the mentioned element
Negative	The calculated correction	**Remove** the mentioned

correction	cannot be explained by Physical laws	element
Unexpected correction	The parameter for the correction is unexpected big.	If the reason can be found and explained, the message can be ignored (2)
No. of Standards too low	Too many corrections No samples selected	More samples or less corrections (including Offset) "Enable" samples
Negative Slope	The slope of the calibration line is negative	Many times, there is an error in the given concentration like a wrong unit during definition. **Has to be removed**

Known examples for error messages which can be explained / ignored:
(1) "Offset seems to be too big" If the detector has a Zirconium collimator, the offset for Zr will generate this message - that's ok.
(2) "Unexpected correction" Some K- and L-series line-overlapping like Ba-L and Ti-K are creating these messages, if they are corrected.

SPECTRO XEPOS XRF Tutorial

31 Method Administration

The term *method* is used in a very specific way in the X-LabPro Software. A *method* is far more than only a calibration.
It is a complex structure built up from sub-methods:

The Method Administration is divided into different parts:

- General
- Elements
- Standards
- Measurement
- Deconvolution
- Calibration
- Output

In *General* all general parameters can be found.

In *Elements* the elements for the calibration (and additional elements, which can be in the samples) are selected.
In addition the concentration range is defined here.

The card *Standards* contains a list of all standard samples in this method. This list is used to create standards, to define the given concentrations...

Measurement defines all parameters of the *measurement*: the x-ray tube conditions (voltage and current), type of sample, evacuation of the sample chamber, measuring time, target, and so on.

The *deconvolution* section defines the elements of interest for each target / measurement.
During the *deconvolution* the net count rates for the selected elements are determined.

The *calibration* contains the functions typically described by the term calibration. The selection of a specific calibration model and the correlation between net count rates and concentrations are part of this sub-method.

This options and cards can be used to modify or check an existing method.

To *create a new method*, a comparable method should be selected in the tree part of the screen. This source is copied using *New* in the menu Method. The visible method is copied (with or without samples can be chosen in the following window). That is the best way to start, because a method contains a lot of parameters and details and all these will be copied from a working method. That's much easier then start to start all over.

"How to create a new Method?" desrcibes the sequence of the most important steps.
In addition to this way, the Method Wizard can be a help to accelerate this.

The a.m. parts are influenced by each other, and the best way to design a new method is to start with *elements*, followed by the *measurement*, the *deconvolution*, the *calibration* and finished with the *output*.
But even the first steps, the selection of elements and the measurement conditions, are already influenced by the aims of the calibration. A brief outline of the steps for an idealized method development is listed below:

1. Select the Elements, which can be in the samples
2. Select the Elements, for which a concentration should be calculated (they have to be a part of the elements selected one step above)
3. Depending on 1. and 2. the Measurement Conditions have to be selected
4. Measure one or several standards without evaluation and use the Spectra Viewer to check 1. - 3.
5. Optimise the measurement conditions depending on the results of 4.: This can be: Vacuum?, gas-flush?, measurement time? or excitation conditions?
6. Define or optimise the deconvolutrion parameters based on 1. and 2.
7. Measure the calibration standards
8. Optimise background spectra for the method
9. Evaluate the samples to get the net count rates
10. Calibrate the method. The procedure, which should be used, depends on the number of elements and the concentration range
11. Evaluate standards again
12. Edit the output sub-method

Some of the steps are very easy to perform, while others require a detailed knowledge of the software.
All of the critical steps will be explained in detail on the linked pages, but it is impossible to explain all of
the basics of x-ray fluorescence spectroscopy in this guide. Please refer to the typical literature on these topics.

32 SPECTRO Calibration - a Hybrid Procedure

This special procedure combines different procedures to get a calibration that works with unknown samples in unknown matrices.

This is possible, because the evaluation is done in the following steps:

1. **Mass Attenuation Coefficient (mac):**
   As *option*, the MAC calibration can be used as first evaluation step. If this is enabled, the Compton peak is used to calculate the mass attenuation coefficient. That's a physical parameter which can be used to calculate the "concentration" of the non-visible part of the sample (Carbon, Oxygen, Hydrogen, Nitrogen...).
2. **Extended Compton Model:**
   The Compton calibration is an empirical calibration. As part of the Spectro-procedure, it is used to calculate start values for the following and final calibration based on Fundamental Parameters. The Compton model is using the intensity of the scattered Compton peak to correct matrix influence.
3. **Fundamental Parameter Model (FP):**
   The FP calibration is the final calibration in the Spectro-procedure and it's a calibration model, which tries to explain the spectra of the sample by physical equations. At the end of this explanation, a theoretical sample is calculated, which shows the same spectra as the measured one.
4. **Normalization:**
   As the final step, the calculated results can be normalized (as *option*). This normalization works in two possible ways:
   - *mac:*
     If the mac-calibration (see 1.) is used, the results are normalized to the sum of the "visible" part of the sample, which is: *100% minus "non-visible" part*. The size of the "non-visible" part was calculated in step 1.
   - *a fix sum concentration:*
     If a fix sum (like "100 %") is defined, the results will be normalized to this. That's an option, which can be used for alloys.

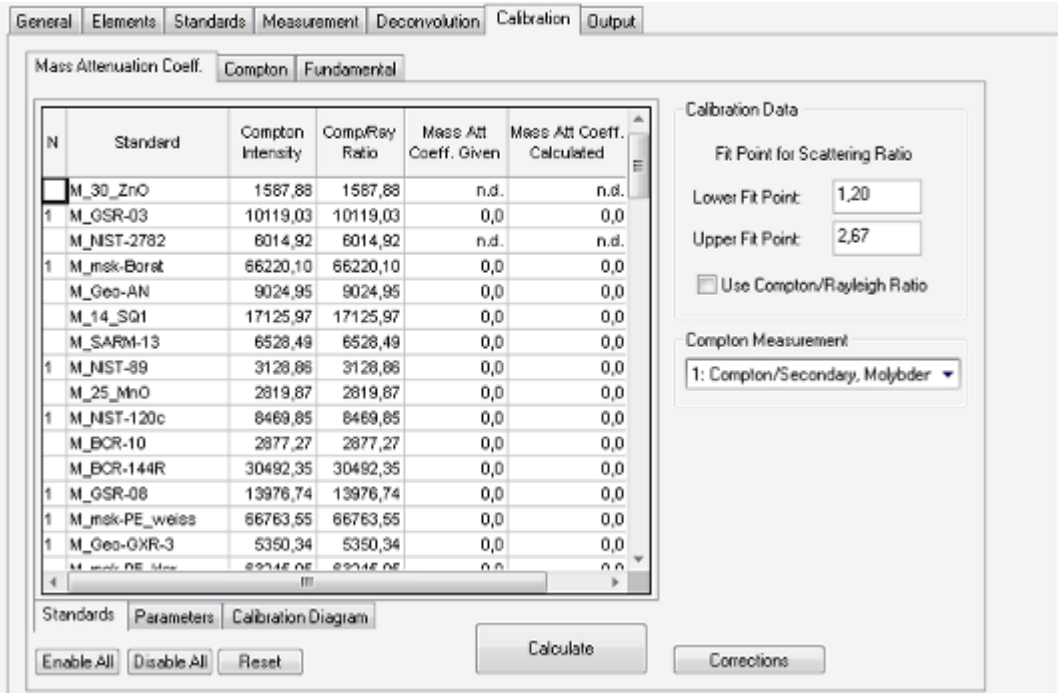
Such a calibration using the Spectro-procedure is done in the following steps:

1. The samples must be **evaluated** to get an intensity for all elements and the Compton peak.
2. The calibration placed on the first tab (*Mass Attenuation Coeff.*) has to be done at first.
3. After finishing this, the samples have to be **evaluated** another time.
4. The next step is, to calibrate using **Compton** procedure
5. After finishing this, the samples have to be **evaluated** again.
6. The last calibration step is the **FPM** procedure.
7. Finally, the samples have to be **evaluated**.

If something is going wrong or if some unexpected results are calculated, an error message appears which informs about the problem.

33 Calibration

The sub-method *Calibration* is used to get the correlation between the measured net count rates and the given concentrations of the standards.
The user interface depends on the procedure which is selected at the tab *General*.



This figure above shows the calibration screen, when the SPECTRO procedure is selected.
This is the most comprehensive calibration and contains three different sub-procedures:

- Mass Attenuation Coefficient This procedure is used to calculate the "concentration" of the non-visible part of the sample. This calculation - based on the Compton-peak - is used to normalize the results (of an unknown sample).
  Whether this feature can be used, depends on the selected procedure.
  Whether it should be used, can be defined in General.
- Compton Calibration This calibration is an empirical calibration. As part of the SPECTRO procedure, it is used to calculate start values for the following and final calibration based on Fundamental Parameters.
  The Compton model is using the intensity of the scattered Compton peak to correct matrix influences.
- Fundamental Parameter Calibration. The Fundamental Parameter Model (FP) is a calibration model, which tries to explain the spectra of the sample by physical equations. At the end of this procedure, a theoretical sample is calculated, which shows the same spectra as the measured one.

  In addition to the SPECTRO procedure both analytical calibrations (Compton

and FPM) can be used separately for calibrations. They can be selected in General.

- On top of this selection list an important and well-known calibration can be chosen:
  Lucas-Tooth, Price. This calibration is the easiest correlation between intensity and concentration, because it's a line, described by *concentration* = *calib-factor* * *intensity*.

As **summary**, three analytical procedures (plus combinations for hybrid procedures) can be used in X-Lab[Pro]:

- Lucas-Tooth, Price as easiest calibration model
- Extended Compton model using the Compton peak for matrix correction, if the concentration range is too wide for Lucas-Tooth/Price
- Fundamental Parameter Model, if the concentration range (and the matrix range) is wide
- SPECTRO procedure as combination of different algorithms. It is used, if the ranges are very wide and the routine samples are completely unknown

33.1 Calibration Procedure

The sub-method *Calibration* is used to get the correlation between the measured net count rates and the given concentrations of the standards. The most simple case is a linear relation between these two values, but in most cases it will be more complex. In X-ray fluorescence, the net count rate is influenced drastically by the matrix and therefore needs an evaluation model to correct for this.

The software X-LabPro contains a wide selection of calibration models. They can be selected using the function *Mathematics* in the tab *General*.

The Calibration models can be divided into three sub-groups:

- Empirical models (like Lucas-Tooth/Price or extended Compton)
- Fundamental parameter models (FPM)
- Specials like Layer Thickness

Fundamental parameter models calculate the inter-element effects on the basis of physical relations. In empirical models, all matrix effects have to be corrected on the basis of real measured standards.
One of the advantages of a fundamental calibration approach is the lower number of necessary standards (approximately one per element calibrated is recommended), but on the other hand the demands on the standards for an FPM are higher. As all inter-element influences are calculated on a theoretical basis the complete composition of a standard, even the concentrations of the elements not measurable via XRF (i.e.: carbon, oxygen), are necessary.
Empirical models are commonly used for narrow ranges of matrix variation or if some other influences, like grain size effects, do not allow the use of fundamental parameter methods.

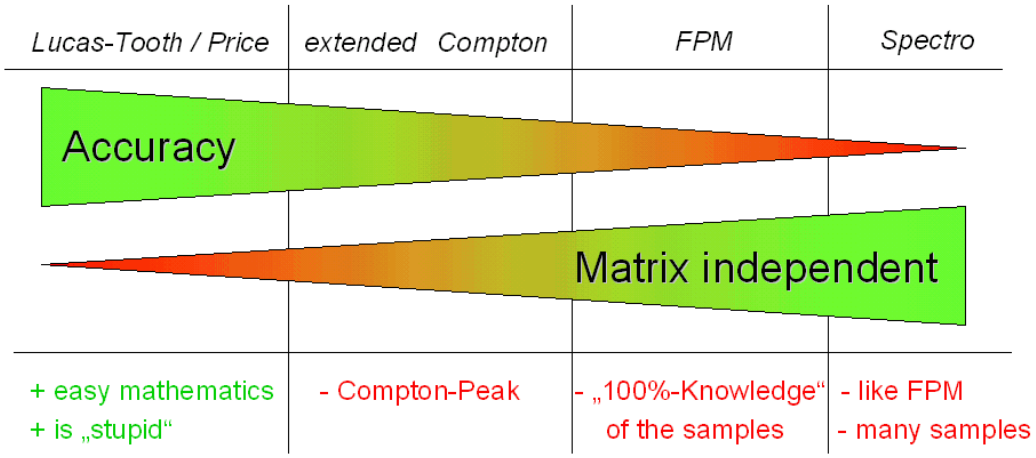
A brief description of the different models, their typical fields of application and some hindrances are listed in the following table:

Calibration Model	Typical Application
Lucas-Tooth, Price	Analysis of low-Z elements (Na to Fe) as main and minor elements. Especially in slag, dusts and minerals when particle size effects hinder a theoretical calculation.
Extended Compton Model	Trace and minor elements (K to U) in low-Z matrix (in some cases even low-Z elements are possible)
SPECTRO procedure	Combination of fundamental parameter and extended Compton scattering model with a calibration of the mass attenuation coefficient. Used for applications like the FPM (thick) model but even if the matrix is unknown and varying like in the analysis of different liquids (oil and water based).
Standard based FP (thick)	Main, minor and trace elements in a varying but known matrix, i.e. additives in oil.
Standardless FP (thick)	As FPM (thick): The normalization to 100% is only useful, if all main and minor elements can be analysed, i.e. alloys.
Standard based FP (thin)	Low sample amount on filter material (i.e. aerosols), very thin films.
Standardless FP (thin)	As FPM (thin): The normalization to 100% is useful, if all of the main and minor elements can be analyzed. Typical application is the rubber technique with diamond paper. The method works without calibration.
ALPHA Normalization Method	Analysis of fused beads with Alpha parameters by de Jongh.
Compton/Rayleigh-Method	Traces in pharmaceutical products, developed by Dr. Schelcher, Hoffmann La Roche.
Layer thickness model	Analysis of the layer thickness on a substrate, i.e. Aluminium on Silicon wafer.

In addition to the calibration models above, some general options can be set here. The calibration models will be explained in the following in more detail.

The following figure compares the four most common procedures with their advantages and disadvantages:

Comparison of calibration procedures



This figure compares the four procedures regarding *Accuracy* and how much they are *matrix indepentent*. The meaning of this comparison is that Lucas-Tooth/Price is the procedure using a minimum of mathematics which results in the best accuracy. The more mathematics are used, the bigger the deviations.
On the other hand, the models located at the left side of this figure, are not able to handle different matrices or a wide range of concentrations in the same calibration. If it is important to use a method, which is matrix independent, one of the models of the right side of the figure should be used.
But then there can be a bigger deviation between expected and calculated results:

In addition, there are some individual advantages / disadvantages for each procedure:

- Lucas-Tooth/Price: The advantage is the simple algorithm. It can be controlled using a pocket calculator and it is "stupid", that means, there are no physical / logical tests (e.g. a concentration can be > 100%) - this can be used for special jobs
- Extended Compton: The most important limitation for this model is the Compton-peak, which is needed. If in measurement no sub-measurement using a Compton-Target is defined, this procedure cannot be used for calculations.
- Fundamental Parameter Model: Defining the given concentrations, the software has to know all information about the elements in the calibration standards, e.g. if a Diesel, containing 400 ppm of Sulphur should be defined, the residual nearly 100 % of "oil" are important for the procedure, too. This 100%-knowledge can be a big problem.
- Spectro-procedure: Disadvantages are the same as for FPM, additionally more samples (especially for mac) are needed.

Unfortunately it is not possible to give a general answer to the question, which procedure should be used.
There are too many details influencing this decision e.g. elements in the samples, concentration range...

One possible way is, to start with the easiest (especially mathemetics) procedure to get an impression about the correlation between intensities amd concentration. If Lucas-Tooth/Price is able to solve this application problem, it's the best choice. If it is not able to solve it, the next procedure can be tried (Ext. Compton, if a Compton-Peak is available). The physical procedures using a lot of mathematics inside should be used at last or if completely unknown samples should be analyzed.

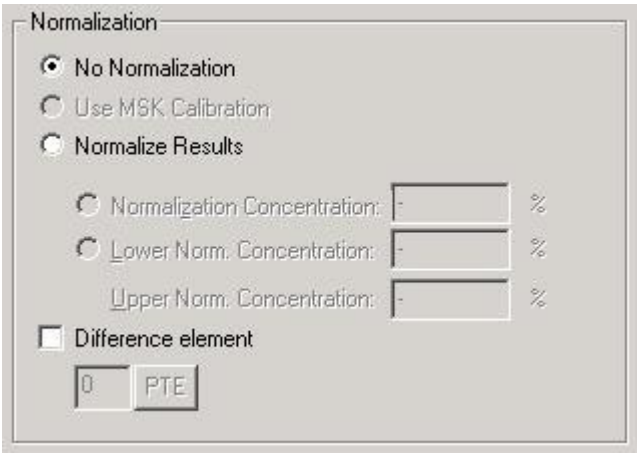
Matrix for Calib. (Element Bonds)

If this option is selected, all elements will be converted to their bonds. This makes it possible to calculate concentrations for low-Z elements (especially Oxygen) without measuring them directly. These calculated values for the low-Z elements will be taken into account during matrix correction.

If Matrix for Calib. should be used, they can be selected in General from a set of predefined bonds. To edit / create predefined *Bonds* the Configuration Editor has to be used.

Normalization

All options for the normalization are concentrated in the *Normailization* region on *General*.
The normalization procedure allows to force the sum of the concentrations on a specific value (defined by *Normalization Concentration*). This function influences the concentrations after the calibration. The options *MSK* (mac) and *Normalization* to a fixed concentration are not possible at the same time. When *MSK* is selected, an additional tab is displayed in the *calibration* tab.
The use of a *Difference element* is an additional option. This can only be one of the non-visible elements (typical H to F). If this option is used the difference between the sum of all analysed elements and 100% is calculated as the difference element. It is possible to select bonds for the difference elements (see sub-method *evaluation*) to define matrices like (CH2)n for an organic sample.



The option Normalize Results normalizes the results before each iteration step, so that the matrix effects are calculated again based on the new information. The option Normalize Results will be performed after the last iteration. This will always lead to a sum of all concentrations equal to the Normalization Concentration. These options can be used successfully, if all elements can be analysed directly (i. e. alloys) or if the bonding state of the elements is exactly known (i.e. oxides in fusions) and the option Matrix for Calib. is selected at the same time.

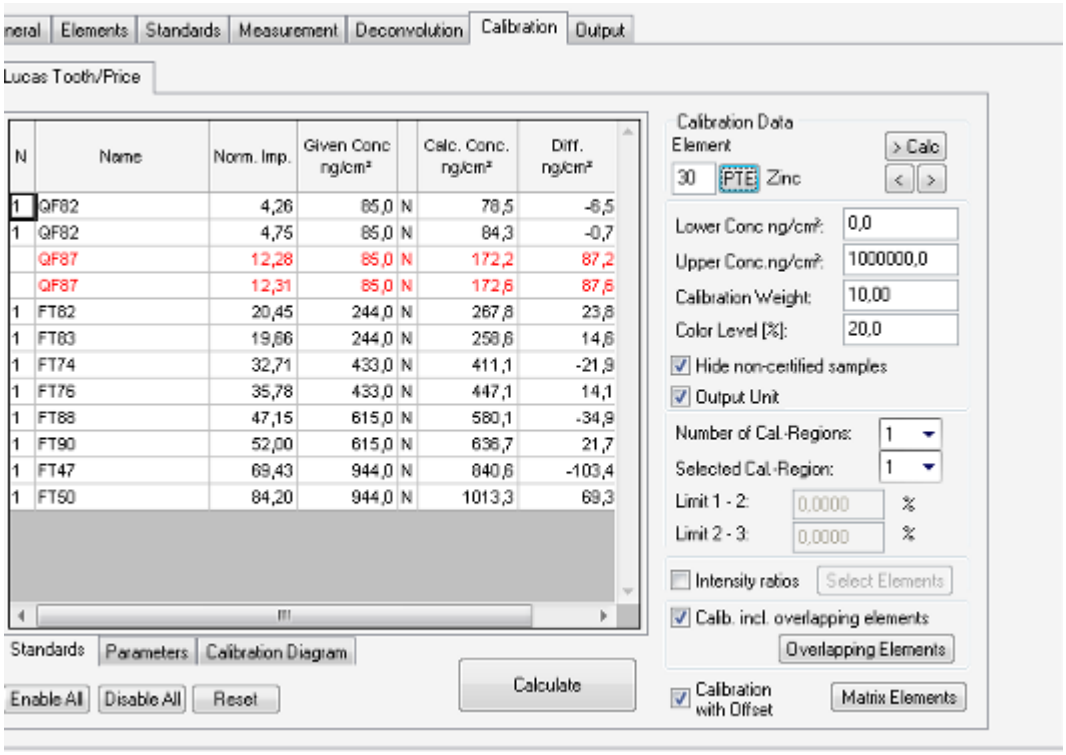
This normalization has nothing in common with the normalization on the Compton scattering peak or the normalization on regions of spectra used in the evaluation process.

33.2 Empirical Calibration using Lucas-Tooth/Price

The easiest possible correlation between intensity and concentration is the following:

$$concentration = calib\text{-}factor * intensity.$$

This describes the procedure called **Lucas-Tooth/Price**.
In detail we find a lot of possible corrections like Offset or 2 types of Interelement-Corrections (Overlapping elements and Matrix elements).



This card shows on the left side the list of the **standard samples**.
There are two possible presentations: If the option *"Hide non-certified samples"* (at the right side) is enabled, two important conditions will control, if a sample appears in this list:
The standard needs a given concentration for this element AND an intensity is found for this element during evaluation.
If this option is disabled, one of these conditions is enough, because it is an OR-condition.

This *standard list* contains different columns:

N	This column shows, if the sample is a part of the calibration and about its weight: **None** Sample is not in the calibration **1-5** The sample is in the calibration. The number shows, how many times this sample will be in the calibration
Name	That's the name of the sample
Norm. Int	The normalized intensity of the selected element in this sample. We like to use normalized intensities, because using them, we are able to handle different tube currents and/or measurement times in the same calibration.
Given Conc.	That's the goal

C	The certification level describes, how "sure" the given concentrations are: **N** Not analyzed. simple: not analyzed **L** Laboratory The given concentration is measured using another instrument **I** Info At a certification paper some values are certified as "Info" **C** Certified The given concentration is certified
Calc. Conc.	The result of the calibration
Diff.	To check the quality of the calibration, the differences between calculated and given concentrations are an important number.

At the right side of this sample list, some options were located, explained in the following:

Lower Conc./Upper Conc.:
These two values were calculated by the calibration mathematics - please do not change them

Calibration Weight

That's a value to control the calibration range, which should be important. If the calibration for smaller concentrations should be increased, reduce the value and vice versa for high concentrations...

Color Level

After the calibration is done the sample are shown using black or red color: The red color means, that the difference between given concentration and calculated value for this sample is too big. The limit, if a line is printed red or black, is this parameter (in % relative).

Hide non-certified samples

This option controls, which samples are shown in the sample list.

Output Unit

The concentrations in the standard list are presented in the internal unit "ppm". Most times it is more comfortable to use the unit, which is used for the printout.

Calibration regions

Only for Lucas-Tooth/Price it is possible, to calibrate using up to 3 regions. If more then 1 region is selected, the limits to switch between the regions have to be defined. The presentation on this card shows only the selected region. As result, the region which is interesting has to be selected. All following steps are now for this region. If another region should be modified, it has to be selected first..

Possible Corrections:

Intensity Ratios

That's an **unusual correction** option, only available for this empirical model (Lucas-Tooth/Price): These are normalized matrix elements (normalization of count rates or weighting of the concentrations). This leads to better analyzes of samples with irregular surfaces. When using this correction, the calibration should be checked with a large number of samples

Overlapping Elements

Elements that influence the deconvolution of the main line of the element of interest through peak overlap. If systematic error occurs (because of this) during deconvolution, the respective elements should be selected here. For example the K-lines of S are overlapped by the M-lines of Pb. This overlapping can lead to a systematic error. Pb should be entered as an overlapping element for S.

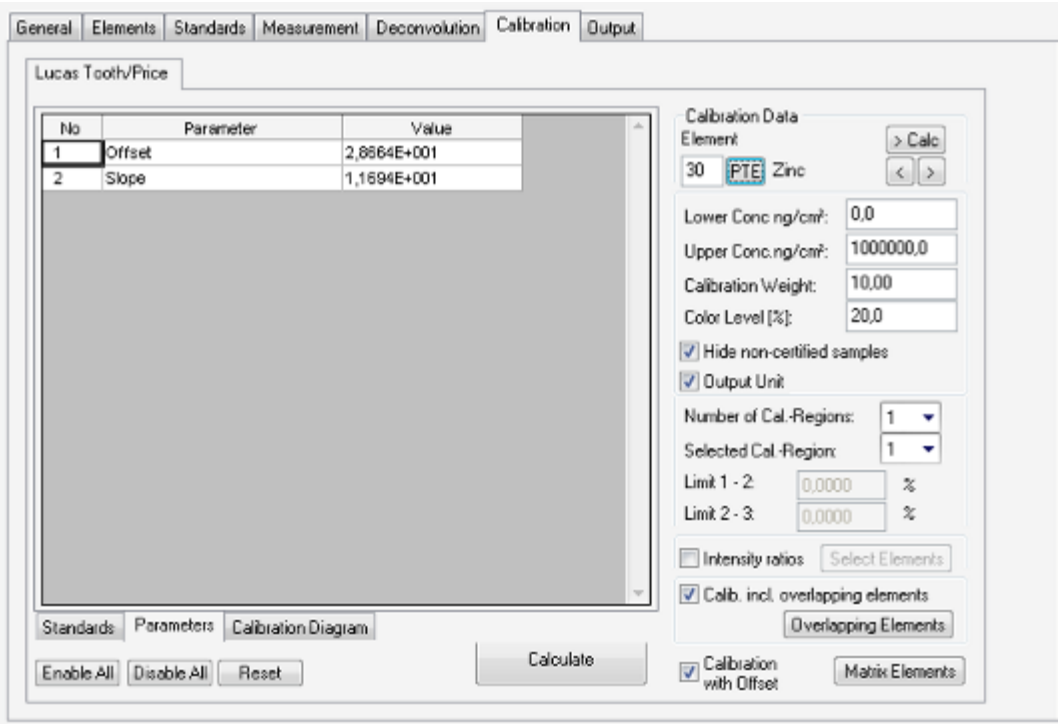
Matrix Elements

Secondary excitation and discontinuity elements are entered as matrix elements for the Compton model. Secondary excitation elements are used for Fundamental Parameter Models. Elements that have a matrix influence on the element of interest are entered for Lucas-Tooth/Price

Offset

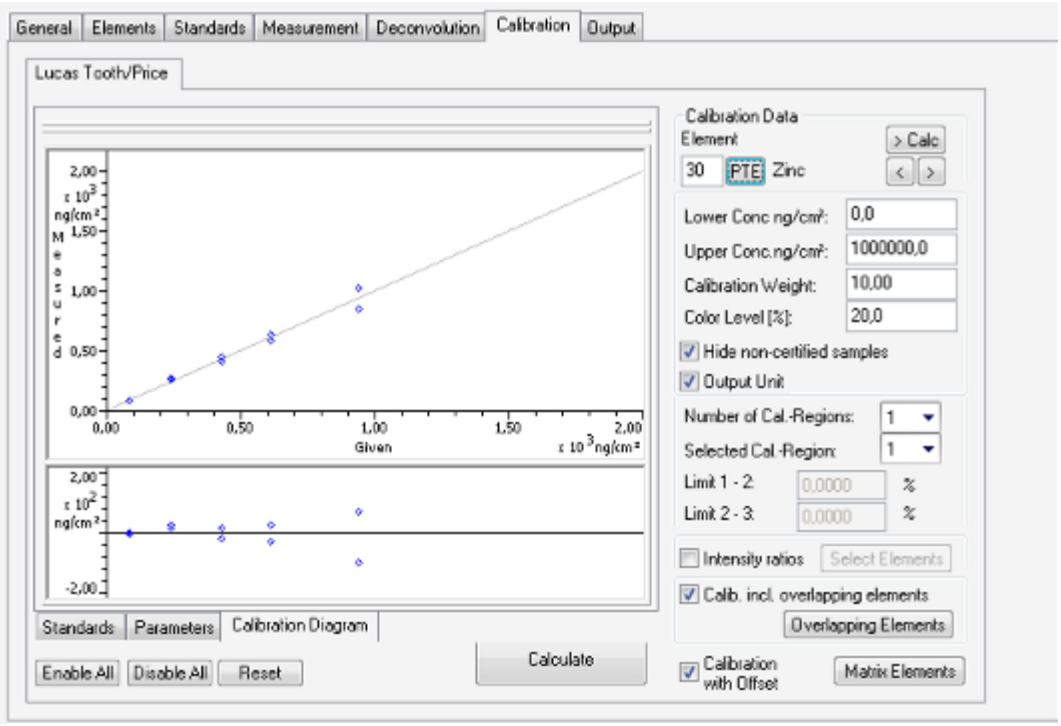
If the calibration needs an offset, this can be enabled here.

Parameters:



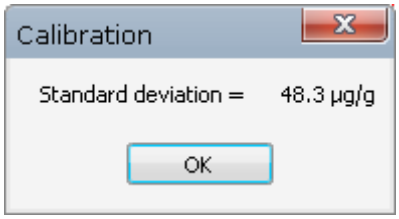
The card *Parameters* shows the calibration parameters.
After a successful calibration the Slope should be shown. All other parameters are additional options.

Calibration Diagram:



The Calibration Diagram shows the calibration line. The different signs are showing the level of certification.
If the right mouse button is used, a context menu is available, to select different options like linear or logarithmic scaling. Touching a sample with the mouse, an info-box appears, that shows some details regarding this sample.
A double-click in the top-line (with the double-line) opens the diagram as full-screen version.

Calculate:



The button Calculate will start the mathematical procedure to calibrate the selected element. If no errors occur, this ends in the window, that informs about the standard deviation during the calibration.

Enable All/Disable All:

A faster way - especially if a complete new method has to be calibrated and each sample is disabled - to enable samples for calibration is the "all"-feature. Instead of

marking each sample individually by clicking, it is much more comfortable to select all samples using this feature.

Reset:

This function allows to reset the calibration to the last set of parameters, if the actual calibration was not successful.

Print:

It is possible to print the calibration data (samples, results, parameters, standard deviation) e.g. for documentation.

If something is going wrong or if some unexpected results were calculated, an error message will appear, which informs about the problem.

33.3 Calibration based on a Fundamental Parameter Model (FPM)

There are two different types of calibrations built-in in X-Lab^{Pro}:

EMPIRICAL CALIBRATIONS and FUNDAMENTAL PARAMETER MODELS

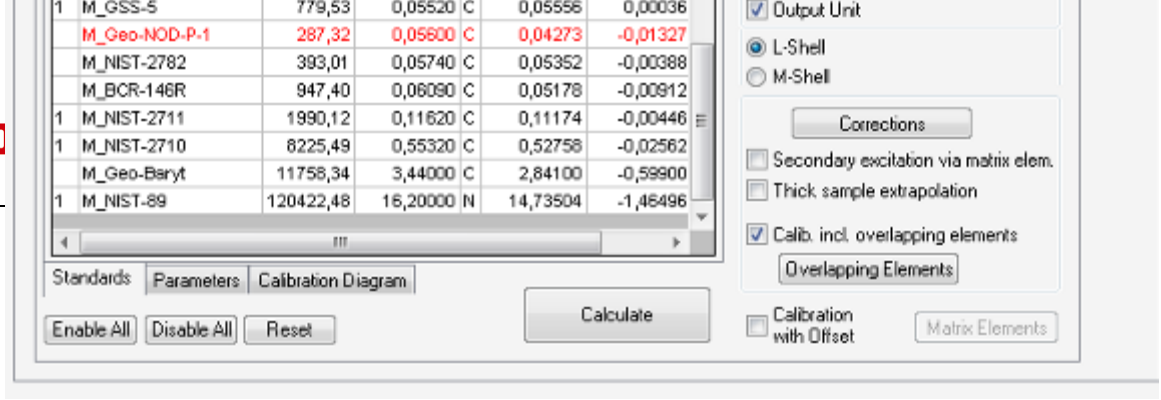
The empirical procedures like extended Compton or Lucas-Tooth / Price try to find a correlation between intensities and concentrations using "stupid" mathematics - if the calculated parameters can be explained or not.

The complete opposite of this strategy are ***Fundamental Parameter Models.*** They try to explain the sample during the calibration and the evaluation of unknown samples. It's not just a calibration factor together with an intensity which are creating the result - it's much more...

During the calibration all known informations about the sample are taken into account. These are much more then the given concentration. These are in addition all other concentrations (including "non-visible" elements like Oxygen), Loss of ignition, the (theoretical) Mass Attenuation coefficient based on the concentrations....

All this together is used for calibration. If the calibration is done and unknown samples are analyzed the evaluation is again not easy, because all calculated information/concentration are used to calculate the element of interest. Unfortunately the concentration of this element can have an influence to other elements.
As result the calculation of the other elements has to be repeated, which will influence again the element of interest....That's a big circle and at the end we will find some concentrations.

The calculated concentrations are responsible for the spectra - that's the theory of the FP-Model.



K-Shell/L-Shell:

That can be an option for future...not available yet.

Secondary excitation via Matrix Elem.:

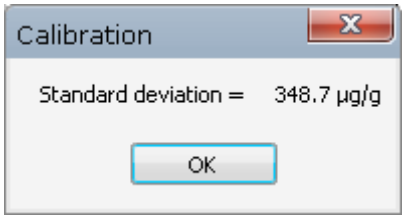
This option allows to work with Matrix Elements, which can be definded, using the "Matrix Elements" icon.

Thick sample extrapolation:

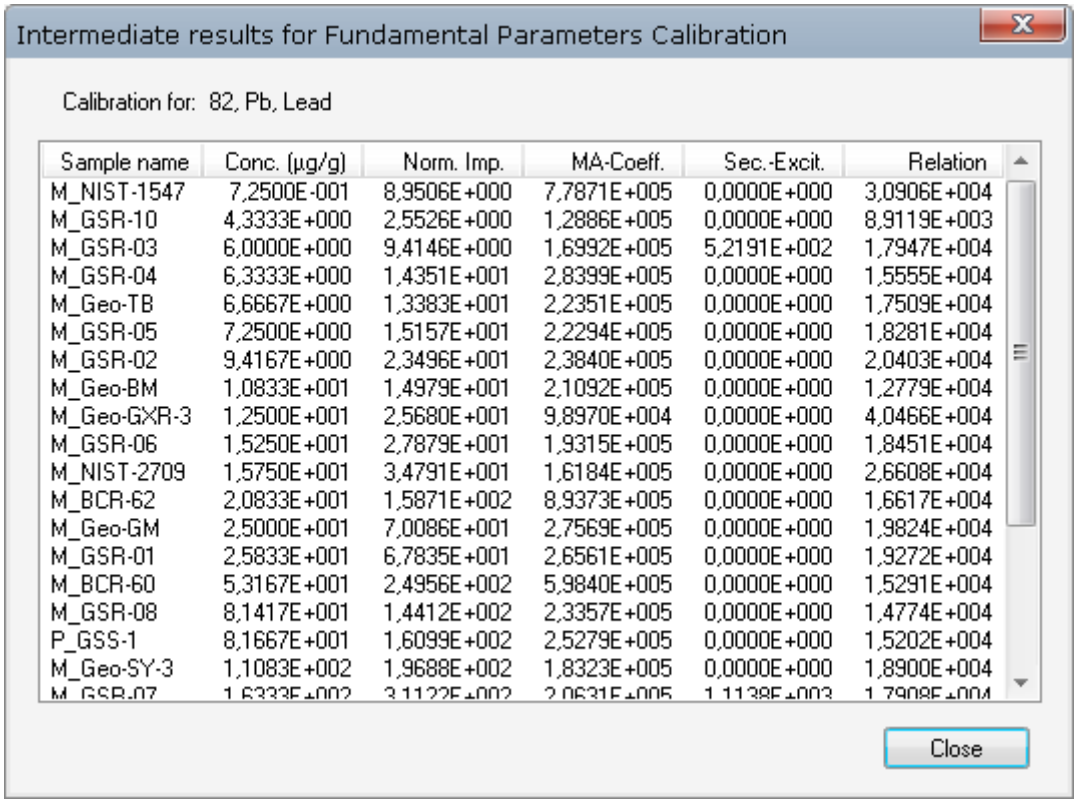
For light elements a sample with a thickness of several millimeters is thick compared to the penetration depth. But the heavier the elements, the bigger the penetration depth of the exciting radiation.
For heavy elements the thickness of the sample influences the intensity in the spectrum.
This parameter uses the sample thickness for calculations. Depending on experience and physical data, this parameter is used starting at Bromine (Br = 35).

Calculate:

after pressing calculate, the calibration is done, but before the final window shows the standard deviation



an additional screen presents some intermediate results:



Sample name	Conc. (µg/g)	Norm. Imp.	MA-Coeff.	Sec.-Excit.	Relation
M_NIST-1547	7,2500E-001	8,9506E+000	7,7871E+005	0,0000E+000	3,0906E+004
M_GSR-10	4,3333E+000	2,5526E+000	1,2886E+005	0,0000E+000	8,9119E+003
M_GSR-03	6,0000E+000	9,4146E+000	1,6992E+005	5,2191E+002	1,7947E+004
M_GSR-04	6,3333E+000	1,4351E+001	2,8399E+005	0,0000E+000	1,5555E+004
M_Geo-TB	6,6667E+000	1,3383E+001	2,2351E+005	0,0000E+000	1,7509E+004
M_GSR-05	7,2500E+000	1,5157E+001	2,2294E+005	0,0000E+000	1,8281E+004
M_GSR-02	9,4167E+000	2,3496E+001	2,3840E+005	0,0000E+000	2,0403E+004
M_Geo-BM	1,0833E+001	1,4979E+001	2,1092E+005	0,0000E+000	1,2779E+004
M_Geo-GXR-3	1,2500E+001	2,5680E+001	9,8970E+004	0,0000E+000	4,0466E+004
M_GSR-06	1,5250E+001	2,7879E+001	1,9315E+005	0,0000E+000	1,8451E+004
M_NIST-2709	1,5750E+001	3,4791E+001	1,6184E+005	0,0000E+000	2,6608E+004
M_BCR-62	2,0833E+001	1,5871E+002	8,9373E+005	0,0000E+000	1,6617E+004
M_Geo-GM	2,5000E+001	7,0086E+001	2,7569E+005	0,0000E+000	1,9824E+004
M_GSR-01	2,5833E+001	6,7835E+001	2,6561E+005	0,0000E+000	1,9272E+004
M_BCR-60	5,3167E+001	2,4956E+002	5,9840E+005	0,0000E+000	1,5291E+004
M_GSR-08	8,1417E+001	1,4412E+002	2,3357E+005	0,0000E+000	1,4774E+004
P_GSS-1	8,1667E+001	1,6099E+002	2,5279E+005	0,0000E+000	1,5202E+004
M_Geo-SY-3	1,1083E+002	1,9688E+002	1,8323E+005	0,0000E+000	1,8900E+004
M_GSR-07	1,6333E+002	3,1122E+002	2,0631E+005	1,1138E+003	1,7908E+004

If something has gone wrong or if some unexpected results are calculated, an error message appears, which informs about the problem.

Corrections:

There are three places to select corrections at this calibration screen:

Overlapping Elements
- Matrix Elements
- Calibration with Offset

33.4 Calibration with Extended Compton Model

Another well known procedure in XRF-calibration technique is the Compton Model. One of the interactions between radiation and material is called Compton effect:
During this **scattering**, a photon will interact with one of the outer electrons of an
atom of the material and doing this it will lose a part of its energy.

Using a secondary target, this energy loss can be observed, because the Compton Peak is visible (at the low-energy side of the peak created by the target material, e.g. Molybdenum).

What's the analytical advantage of the scattered Compton Peak?

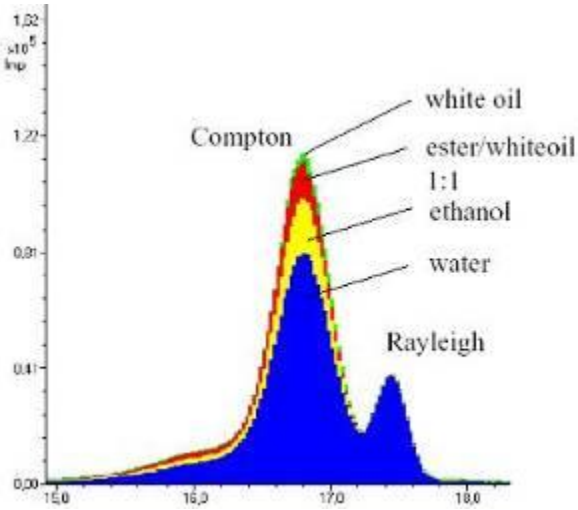
The easiest empirical procedure (Lucas-Tooth/Price) has the disadvantage, that it will work only properly, if the concentration range is limited and the matrix is the same for all samples (in detail both limitiations have the same meaning, because a wide range of concentrations will influence the matrix...). The wider the concentration ranges in the matrix, the poorer the quality of such a Lucas-Tooth/Price calibration.

The Compton model is using the intensity of the scattered Compton peak to correct for matrix influences.

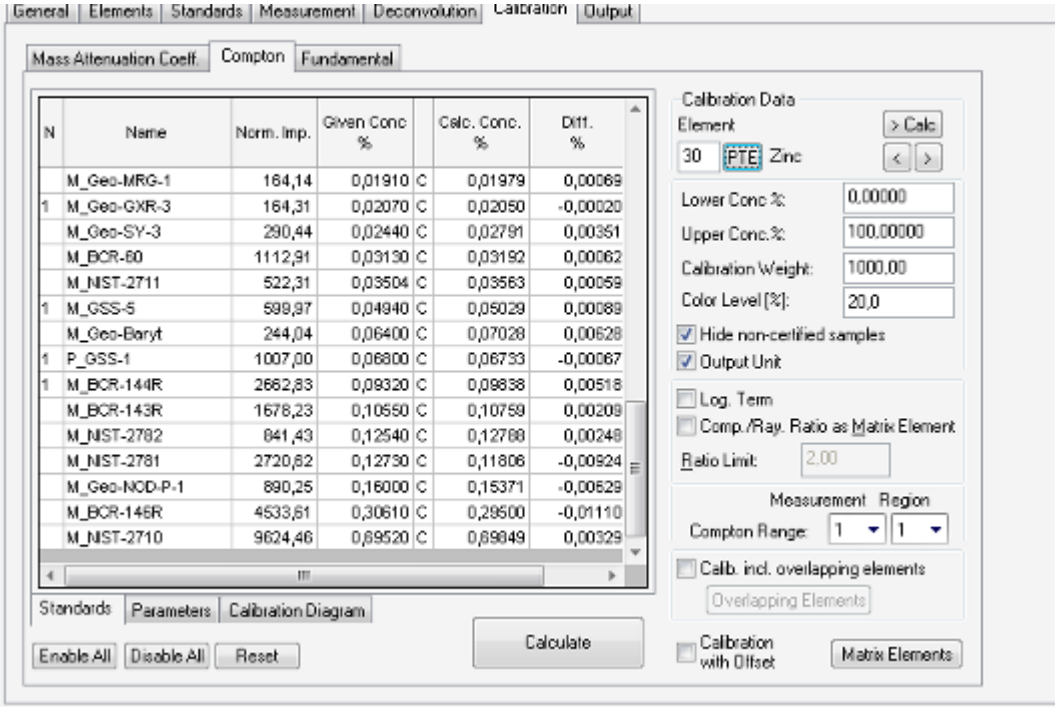
This is working, because the Compton intensity depends on the "heaviness" of the sample:

Light samples (like organic samples) have a big Compton peak and heavy samples (like ores or metals) have a small Compton peak (see end).

This figure compares the Compton peaks for different solution materials.
The bigger the Oxygen part in the chemical bond, the smaller the Compton peak, because water (shown in blue) is heavier than oil (in green) without any Oxygen.



This effect is used to calculate a matrix correction, which allows to calculate a calibration with different matrices and/or with a wider concentration range (because a wide concentration range is similar to different matrices), compared with Lucas-Tooth/Price. The disadvantage of this correction is an additional mathematical step, which will increase the statistical error in the calibration, because now two intensities (element and Compton) instead of one (only the element in Lucas-Tooth/Price) are used. Each intensity has its own error (statistical and
mathematical caused by deconvolution) and that's the reason, why the error of a Compton calibration is higher compared to Lucas-Tooth/Price.

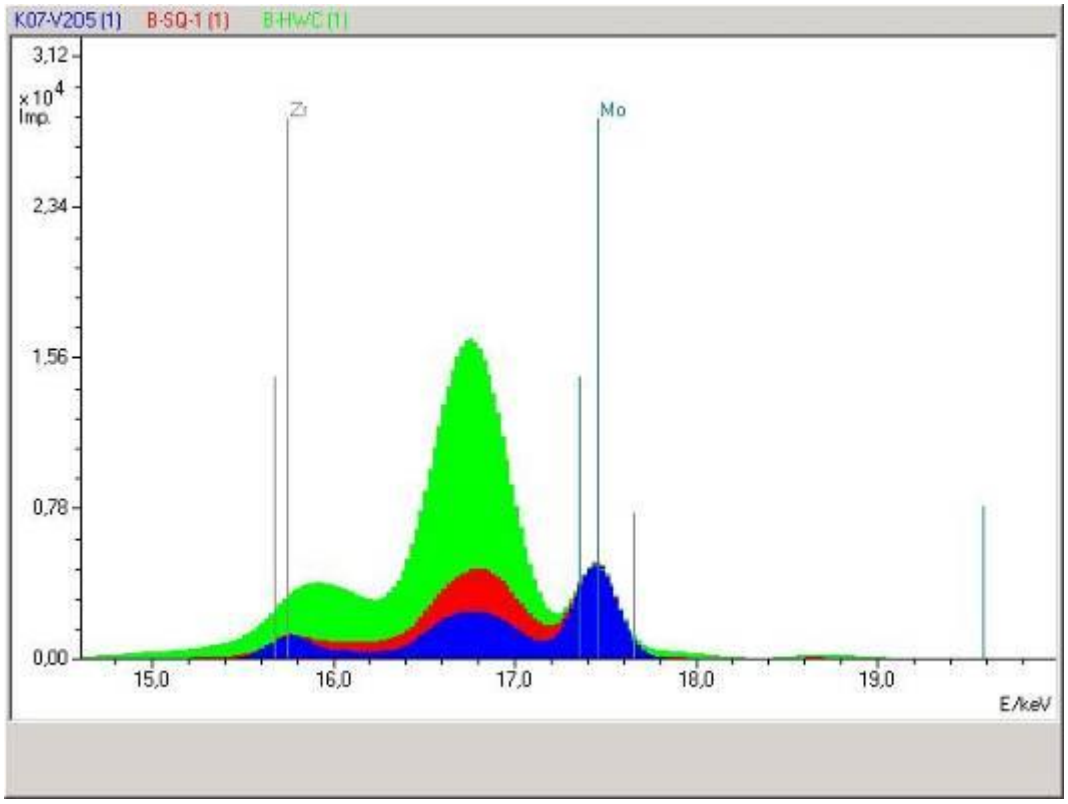


This figure shows the tab for the Compton calibration. In the following only the differences to the same screen in Lucas-Tooth, Price are presented,. These differences are located at the right side of the tab:

- 2 or 3 calibration regions are not available
- Log. Term: hat's an additional calibration parameter that can be used in this procedure.
- Comp./Ray. Ratio as Matrix Element: The ratio Compton/Rayleigh is used as internal standard to normalize results. This feature can be used for light matrices (organic) with a big Compton peak.
- Compton Range: These 2 numbers describe in which measurement (here the first one) the Compton-peak is found. The second number is the number of a region (ROI) selected in the deconvolution - do not modify these entries.

If something is going wrong or if some unexpected results were calculated, an error message will appear which informs about the problem.

This final figure shows the above mentioned differences between light, mid-range and heavy matrices:

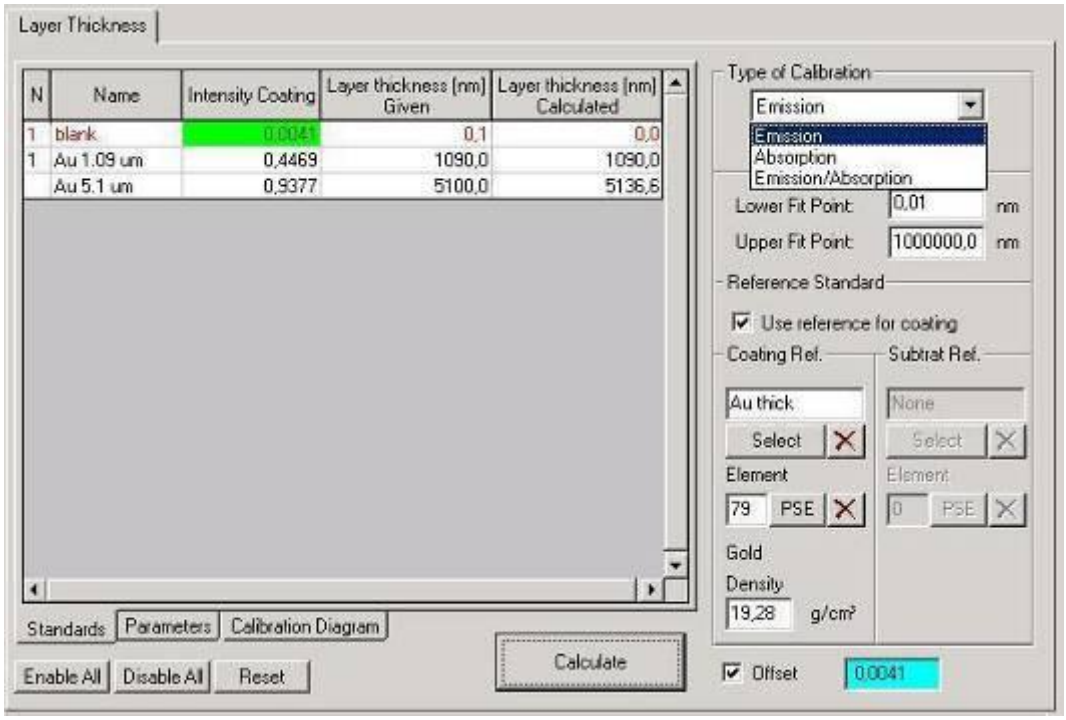


This figure shows the big differences in the Compton intensity for
- Wax (Organic Matrix = green)
- a glass sample (SiO2 = red)
- V2O5 as a heavy oxide sample (blue)

33.5 Special procedure for Calibration of Layer thickness

Analysis of the layer thickness on a substrate, e.g. Aluminium on Silicon wafer or layers of Gold.

The tab looks different compared to the other procedures, because this calibration is a special one:



First of all a layer thickness can be detected in different ways:

- The Emission of the coating is detected and the thicker the coating is, the higher the intensity.
- The second way is Absorption: The observed intensity is created by the substrate.
  The thicker the coating is, the bigger the absortion of the radiation of the substrate and
  the smaller the intensity of the observed peak of the substrat element.
- The best way is a combination of both: Emission/Absorption

The first calibration can be used for Au-Layers on other metals, the second can be used, if the coating material is not visible for XRF (like plastic coatings) and the combination is used e.g. for wafers.

The example above shows case 1 (Emission of the coating material) for Gold layers. In this case some options for the substrate material are disabled, because the substrate is not taken into account.

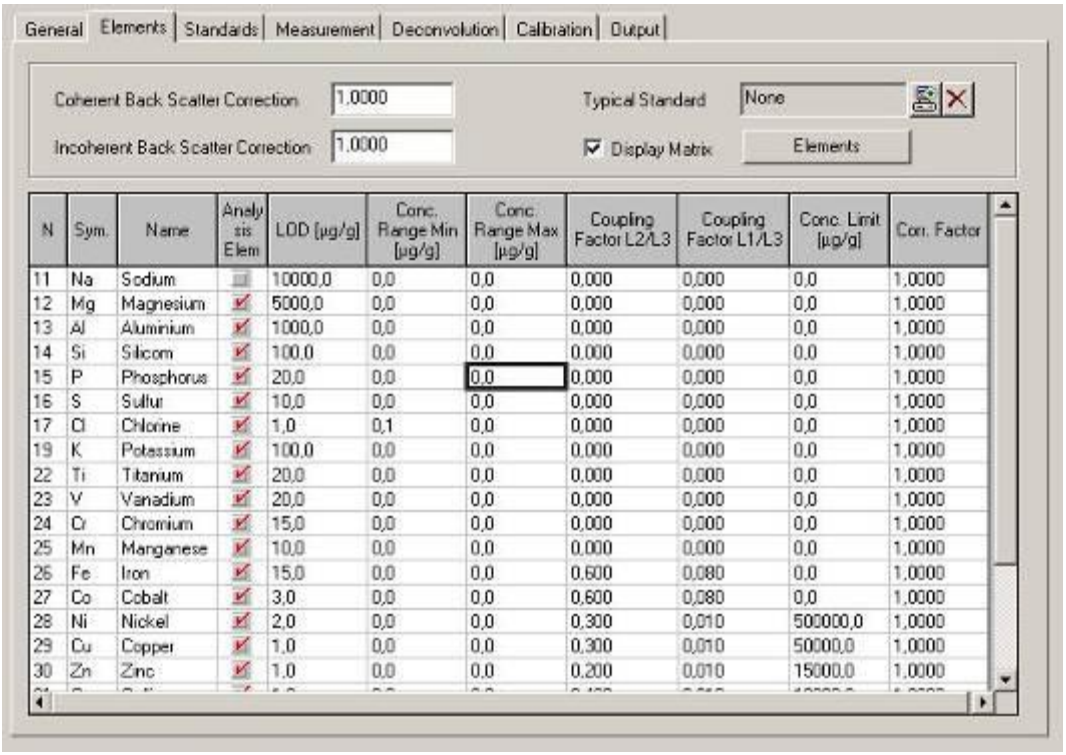
The calibration is completed, if the intensity, which is found for the blank sample (green high-lighted in the figure above), is used as "**Offset**" value (here: 0,0041) (light blue). **This has to be done manually !!!!**

33.6 Elements

This tab is one of the most important tabs in a method, because it contains a list of all elements, which

a) can be contained in the samples
b) should be analyzed.

Both will control the Measurement Conditions and the Deconvolution!



N	Sym.	Name	Analysis Elem	LOD [µg/g]	Conc. Range Min [µg/g]	Conc. Range Max [µg/g]	Coupling Factor L2/L3	Coupling Factor L1/L3	Conc. Limit [µg/g]	Corr. Factor
11	Na	Sodium		10000,0	0,0	0,0	0,000	0,000	0,0	1,0000
12	Mg	Magnesium	✓	5000,0	0,0	0,0	0,000	0,000	0,0	1,0000
13	Al	Aluminium	✓	1000,0	0,0	0,0	0,000	0,000	0,0	1,0000
14	Si	Silicon	✓	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
15	P	Phosphorus	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
16	S	Sulfur	✓	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
17	Cl	Chlorine	✓	1,0	0,1	0,0	0,000	0,000	0,0	1,0000
19	K	Potassium	✓	100,0	0,0	0,0	0,000	0,000	0,0	1,0000
22	Ti	Titanium	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
23	V	Vanadium	✓	20,0	0,0	0,0	0,000	0,000	0,0	1,0000
24	Cr	Chromium	✓	15,0	0,0	0,0	0,000	0,000	0,0	1,0000
25	Mn	Manganese	✓	10,0	0,0	0,0	0,000	0,000	0,0	1,0000
26	Fe	Iron	✓	15,0	0,0	0,0	0,600	0,080	0,0	1,0000
27	Co	Cobalt	✓	3,0	0,0	0,0	0,600	0,080	0,0	1,0000
28	Ni	Nickel	✓	2,0	0,0	0,0	0,300	0,010	500000,0	1,0000
29	Cu	Copper	✓	1,0	0,0	0,0	0,300	0,010	50000,0	1,0000
30	Zn	Zinc	✓	1,0	0,0	0,0	0,200	0,010	15000,0	1,0000

As first step (using the button *Elements* on top) all possible elements have to be defined.
These are the elements which can be in the samples.

All the selected elements are visible in the list, shown above. Now, as second step, one can assign the elements of interest. This can be done by using the *Analysis Elem* column.
If an element is marked here, the intensity of this element is fed to the calibration procedure to calculate a concentration.

The LODs are the Lmits Of Detection for each element.

The column *Conc. Range Min. [µg/g]* defines the lower limit of the calibration and it describes the detection limit. The following column *Conc. Range Max. [µg/g]* is important to define the size of the concentration range. That's an important information regarding the calibration procedure. The values for both columns will be extracted from the method automatically.

Whether the columns called *Coupling Factor L...* and *Conc. Limit [µg/g]* are visible, depends on the user level.

The last column contains the correction factors, which are calculated during a Method Recalibration.
In addition to these factors the two factors for the scattering intensities (*Coherent Back Scatter Correction* and *Incoherent Back Scatter Correction*) are editable on top of the list.

If Bonds should be used, they can be selected from a set of pre-defined bonds at General and/or Output.
To edit / create pre-defined bonds the Configuration Editor has to be used.

33.7 Measurement

The setting of the measurement conditions is one of the first steps of the method development. It is necessary to decide the purpose of the method first. Which are the critical parameters, detection limits or measuring time?
Is it possible to measure the samples in vacuum or is gas flushing necessary?
Which elements are important?

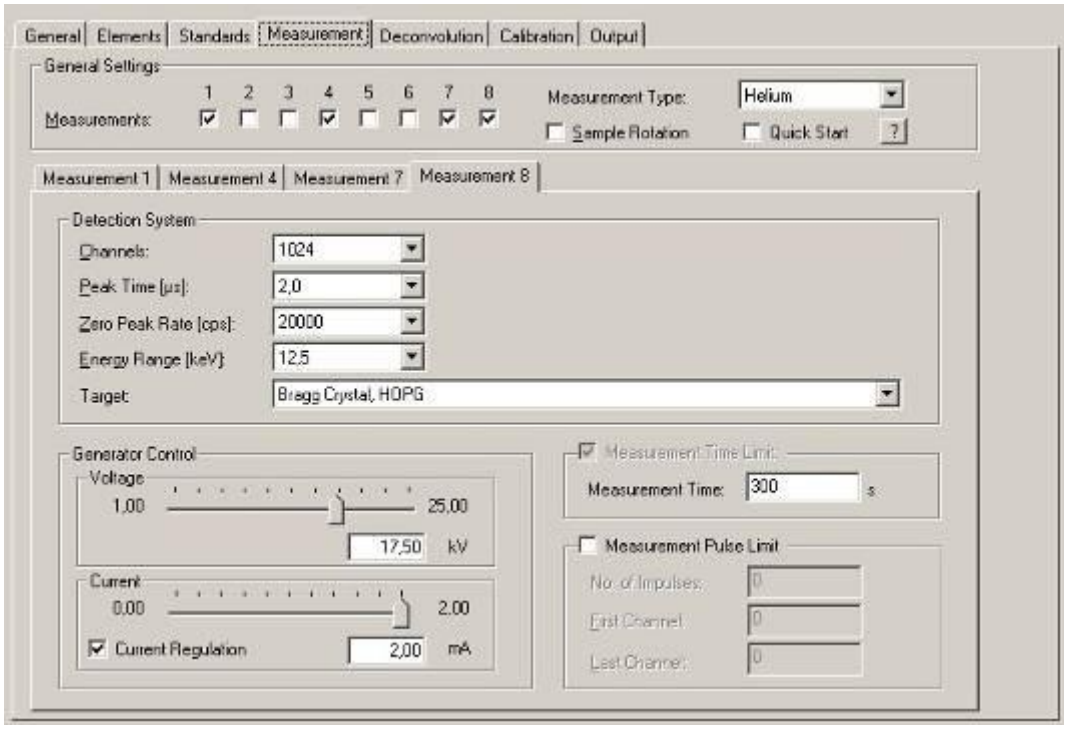
These questions have to be answered in advance to create a tailor made method for a specific application.

For almost all elements a variation of different excitation conditions exists for each instrument. The first step is to select the best target combination for a specific method.
A method is limited to 8 different targets. The number of targets used is influenced by the analytical needs and by the measuring time.

Some basic rules for the development of a measurement strategy:

1. Always start the method with the Compton target if you need the information of the Compton Scattering (for details: see Calibration).
2. Proceed with the target requiring the highest excitation energy. The information from this measurement about the concentration of the heavy elements can be used to improve the deconvolution of low-Z elements influenced by line overlaps of the L or M-Lines of the heavy elements.
   Such a combination is Molybdenum and Sulphur: The Sulphur-K-line, which is used for calculations, is overlapped with the Mo-L-line.
   Without any correction, Mo in the samples will influence the S-results. If the sub-measurement which calculates Mo-K is done before the S measurement the result of the latter can be corrected.
3. To analyze traces of light elements in a high-Z matrix, use a target that can only excite the analyte. This is only possible if the energy of the excitation source is between the absorption edges of analyte and matrix.
4. To increase the count rate, it is possible to increase the tube current. Increasing the tube current leads to a higher intensity of the radiation. Increasing the tube voltage not only changes the intensity, but also the spectral composition of the radiation. Thus, it is necessary to create new background spectra when the tube voltage is changed.

All measurement parameters are set in the sub-method *Measurement*.



The *General Settings* of the measurement are located in the upper half of the screen. The number of sub-measurements can be selected here. Additionally, the environmental conditions (vacuum, air or He-flush) are selected here.

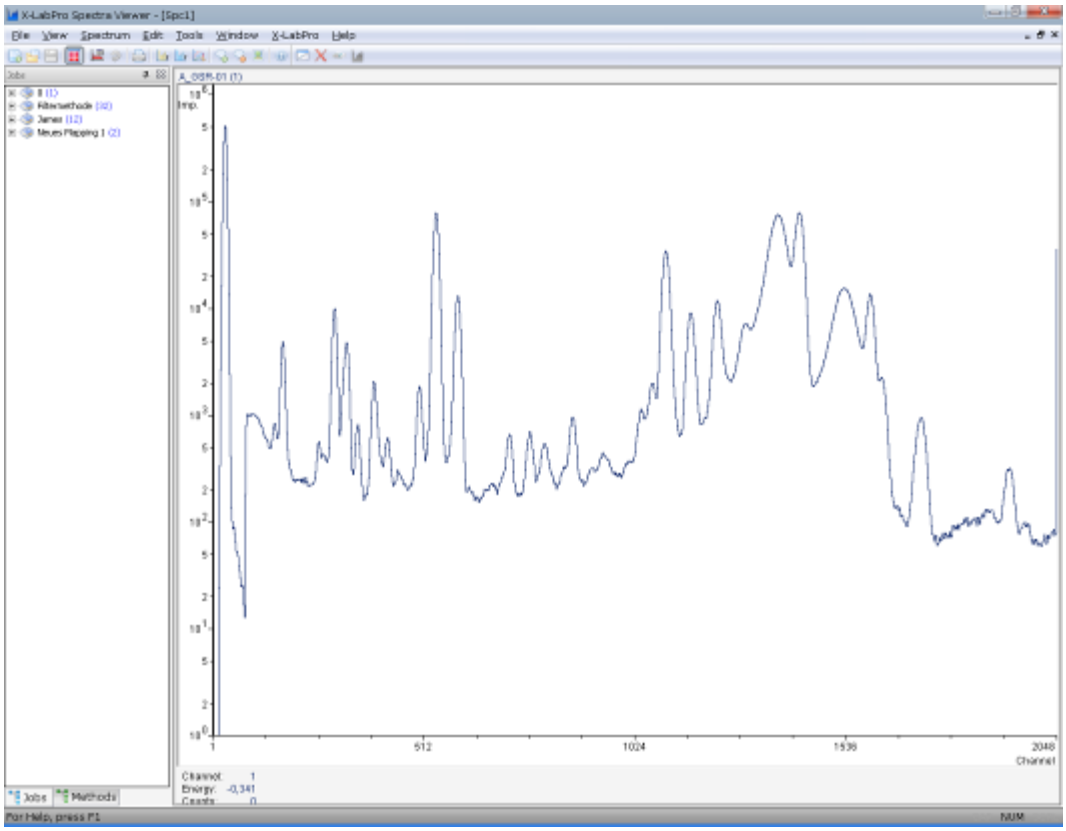
The lower half of the screen contains the settings of sub-measurements for this method.

Some of the values in the lower part of the window should not be changed, others can be varied (see below). An overview of the parameters, the possible settings are listed in the table below.

Parameter	**Notes**
Channels	1024 and 2048 channels are recommended for measurements at the *Energy Range* 12,5 and 25 keV, respectively. For measurements at the the *Energy Range* of 50 keV 4096 channels should be used. - **Do not change**
Peak Time [µs]	The time for the detection electronics to shape a peak. This time is a characteristic value for the detection electronics. It is important to note that all used combinations of *peak time* and *energy range* must be calibrated with the Method called MCA. - **Do not change**
Zero Peak Rate [cps]	Necessary for the accurate dead time correction - **Do not change**.

Energy range [keV]	The scaling of the x-axis of the spectra. For light elements we like to use 12.5 keV, for mid-range energies 25 keV and for heavy elements 50 keV. Each target or filter has its own recommended Energy range. - **Do not change**
Target	Selects the target for this sub-measurement.- **Do not change**
Voltage	The excitation depends on the voltage which ist used. A voltage depending on the selected target/filter is recommended. Changes in the voltage will influence the background spectra which have to be modified after changing the voltage. - **Do not change**
Current	The optimum dead time is 25%. If *Current Regulation* in enabled (see next item), the current stored here is only the default start value. This will be regulated depending on the intensity which is influenced by the sample type.
Current Regulation	When this option is activated, the settings for tube current will be used as a starting current only. The software will measure the sample with the given settings and then optimize the tube current. The resulting intensity should not exceed 100,000 cps.
Measurement Time Limit	Default: This option is selected as standard stop criteria.
Measurement Time	This is the clock time for the measurement. It is not possible to select a live time. Live time = clock time * (1 - rel. dead time).
Measurement Pulse Limit	An alternative option to end a sub-measurement. If the number of counted impulses is bigger than the given value in *No. of Impulses* the measurement will stop. If both options (*Measurement Time Limit* and *Measurement Pulse Limit*) are selected, the criteria first met will stop the sub-measurement.
No. of Impulses	For the *Measurement Pulse Limit* option the criteria for stopping the sub-measurement can be set here.
First Channel	For the above listed option *No. of Impulses* the region of interest (ROI) must be defined. This is done with the two parameters *First Channel* and *Last Channel*. This is only necessary, if the option *Measurement Pulse* is used.
Last Channel	See above.

33.8 Spectra Viewer

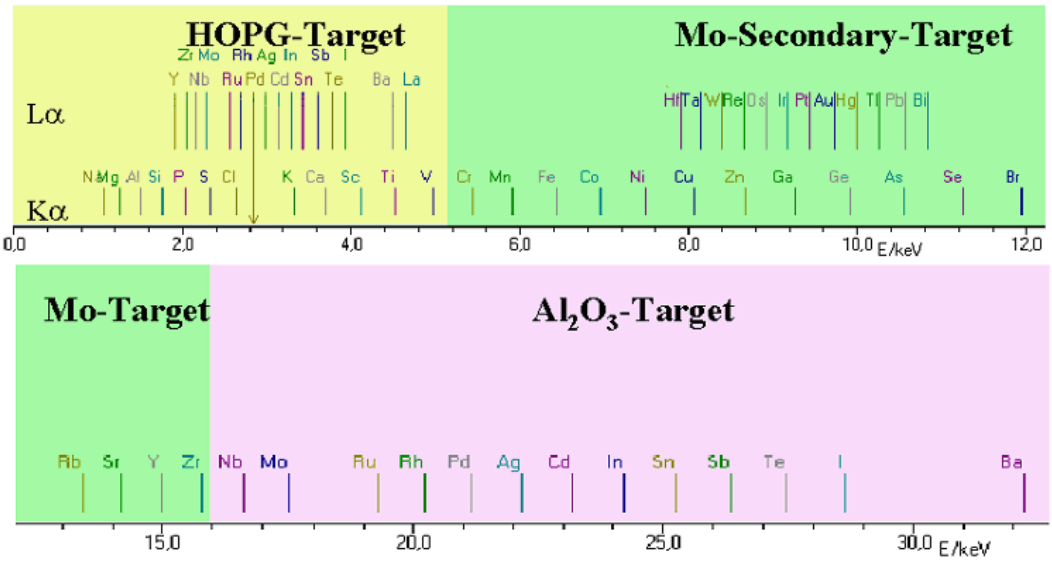


If elements should be identified using only the Spectra Viewer, please take care of the ARTEFACTS !

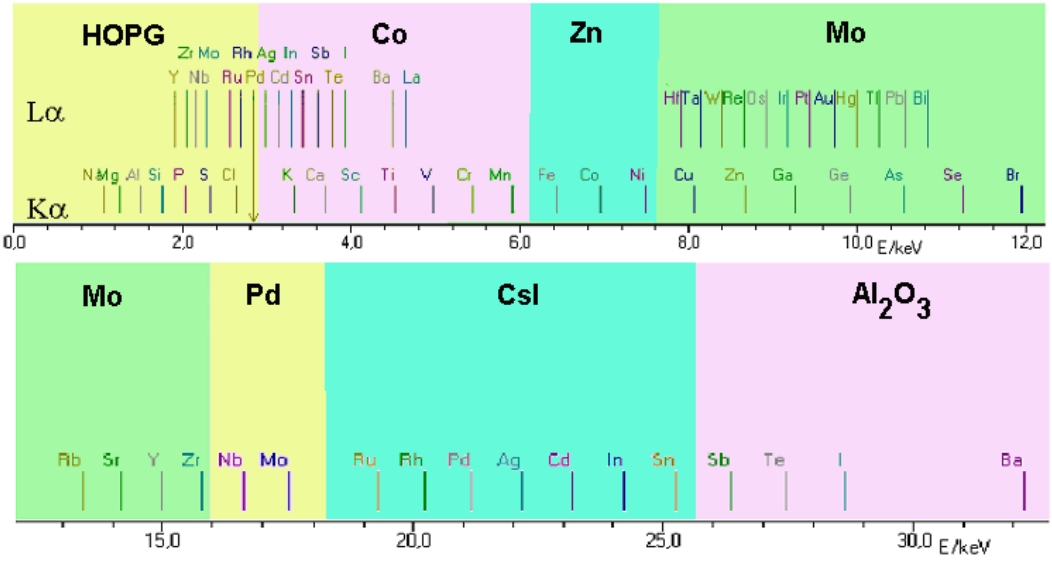
The Spectra Viewer can be used for method development, because the question, which elements could be in routine samples, can be answered a little bit easier using this tool.

This information is necessary to define the deconvolution together with the measurement conditions.

The following figure shows with which target one can calculate which element (for XEPOS and the standard TurboQuant applications).



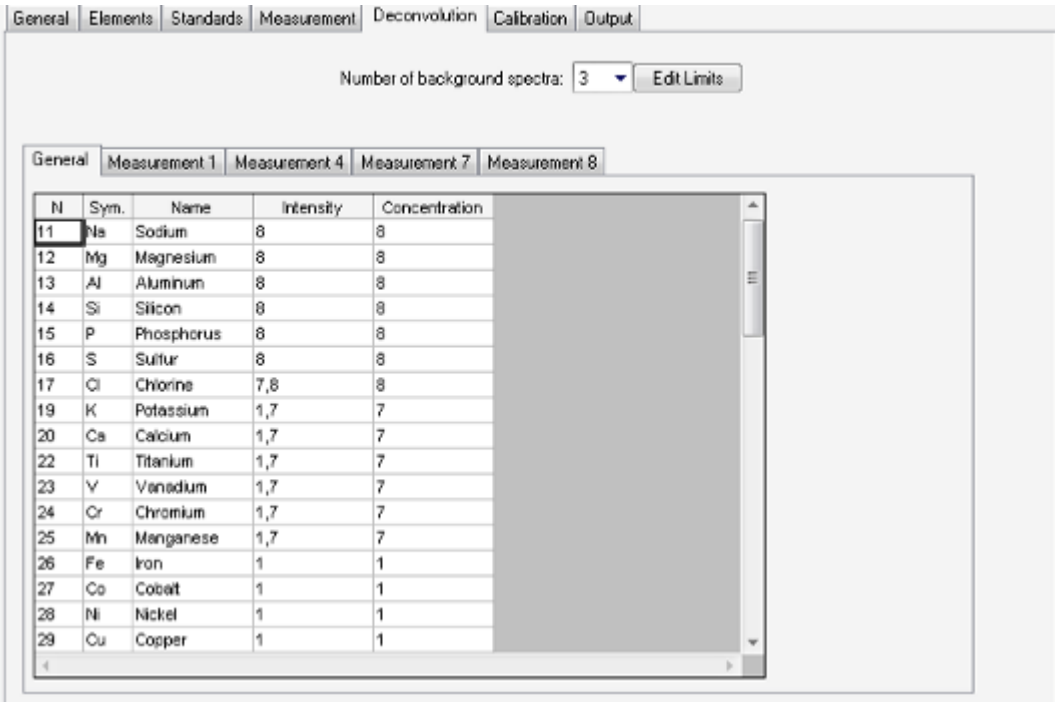
Enhanced TurboQuant conditions using additional secondary targets:



33.9 Deconvolution

The deconvolution is necessary to determine the net counts for the individual elements of the method. This includes the subtraction of a background spectrum and a selection which lines should be used for the deconvolution. As a method is constructed of several sub-measurements, the parameters have to be defined for each of the sub-measurements. It is possible to deconvolute elements in several sub-measurements to correct for line overlaps, but it is only possible to calculate the concentration from a single sub-measurement.

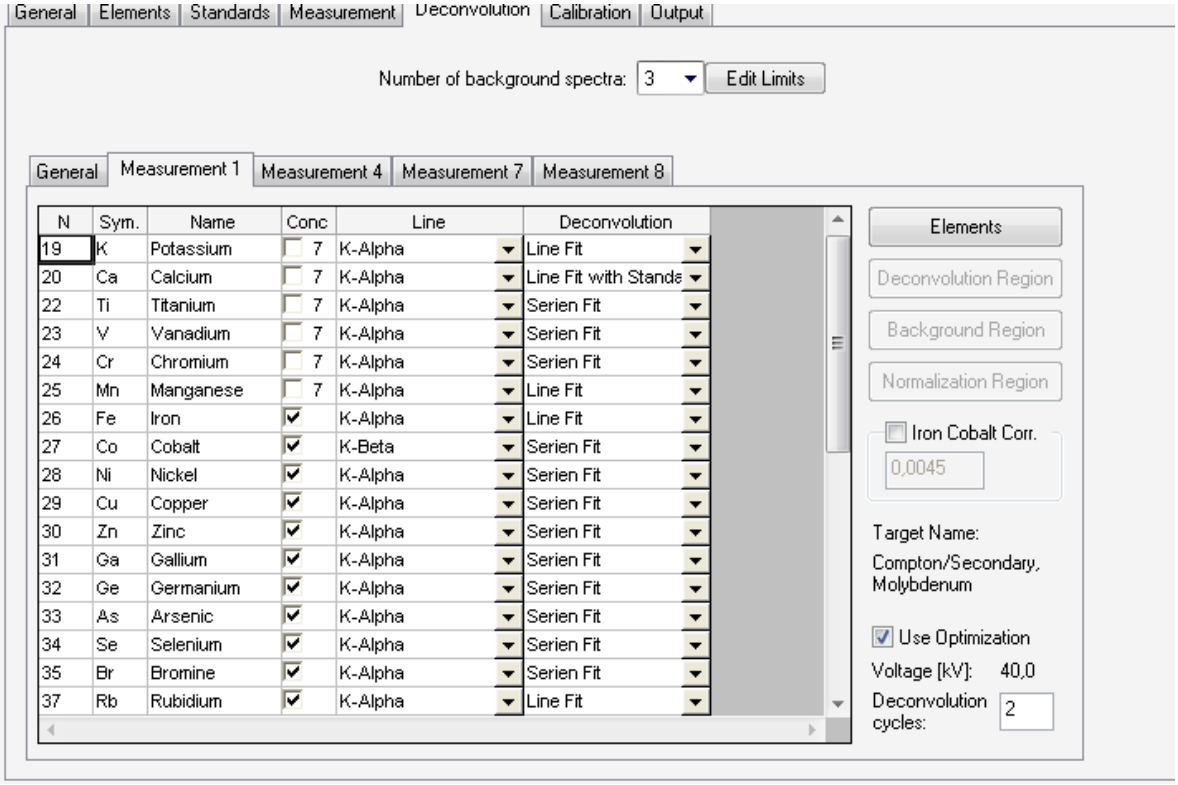
The sub-method *Deconvolution* is divided into two kinds of tabs:
The tab *General* is a summary of the deconvolution to get an overview.



N	Sym.	Name	Intensity	Concentration
11	Na	Sodium	8	8
12	Mg	Magnesium	8	8
13	Al	Aluminum	8	8
14	Si	Silicon	8	8
15	P	Phosphorus	8	8
16	S	Sulfur	8	8
17	Cl	Chlorine	7,8	8
19	K	Potassium	1,7	7
20	Ca	Calcium	1,7	7
22	Ti	Titanium	1,7	7
23	V	Vanadium	1,7	7
24	Cr	Chromium	1,7	7
25	Mn	Manganese	1,7	7
26	Fe	Iron	1	1
27	Co	Cobalt	1	1
28	Ni	Nickel	1	1
29	Cu	Copper	1	1

The number of background spectra and the corresponding switching limits can be selected here. The switchover values are the Compton to Rayleigh scattering ratios. Therefore, it is only possible to use several background spectra, if a Compton target is used in the method. With several background spectra available for each target it is possible to calibrate different matrices with a different scattered background (like organic and silicate samples) in one method.

The list shows which elements have to be deconvoluted during evaluation in general. These elements can be selected at the tab Elements.
All elements which are present in a specific sample, should be selected. Even if the calculation of the concentration is not planned, it may be necessary to deconvolute the lines because of possible interferences and line overlaps.
Using the tabs *Measurement x*, all details of the deconvolution can be modified:



The main part of the screen is a list of elements, which shows all selected elements, using the button Elements at the right side. The elements, which can be chosen at this place are pre-defined on the Elements tab. Only elements chosen on the tab are selectable here.

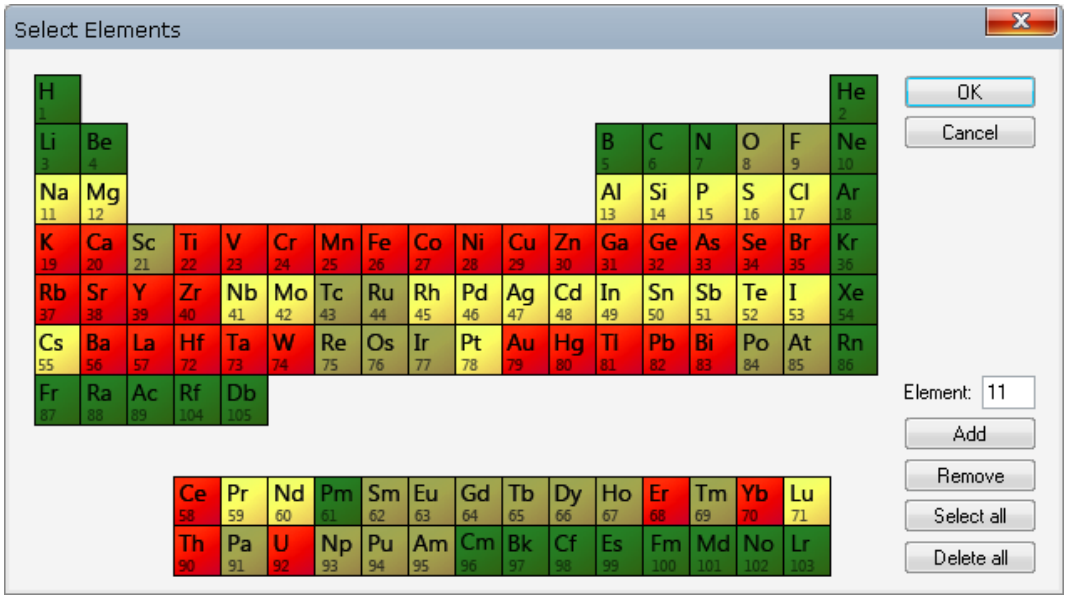
If an element appears in the list, the last three columns can be modified / defined:

The columns *Line* and *Deconvolution* describe the kind of calculation, which should be applied. For example, Sodium will be calculated from the K-Alpha line using *Serial Fit* as strategy. Possible strategies are:
- Summation,
- Series Fit ,
- Line Fit and
- Line Fit with Standardization

The check boxes in the column *Conc* are necessary to decide, whether an intensity is used for the calculation of the concentration or just as intensity e.g. for overlapping corrections. When a number is shown (like for Chromium) that means that the concentration for this element **must be** calculated using the intensity from a different sub measurement (Cr = 1).

On the right hand side there are 4 buttons to edit additional parameters.

Elements
If this button is selected a window with a periodic table of the elements will appear on the screen:



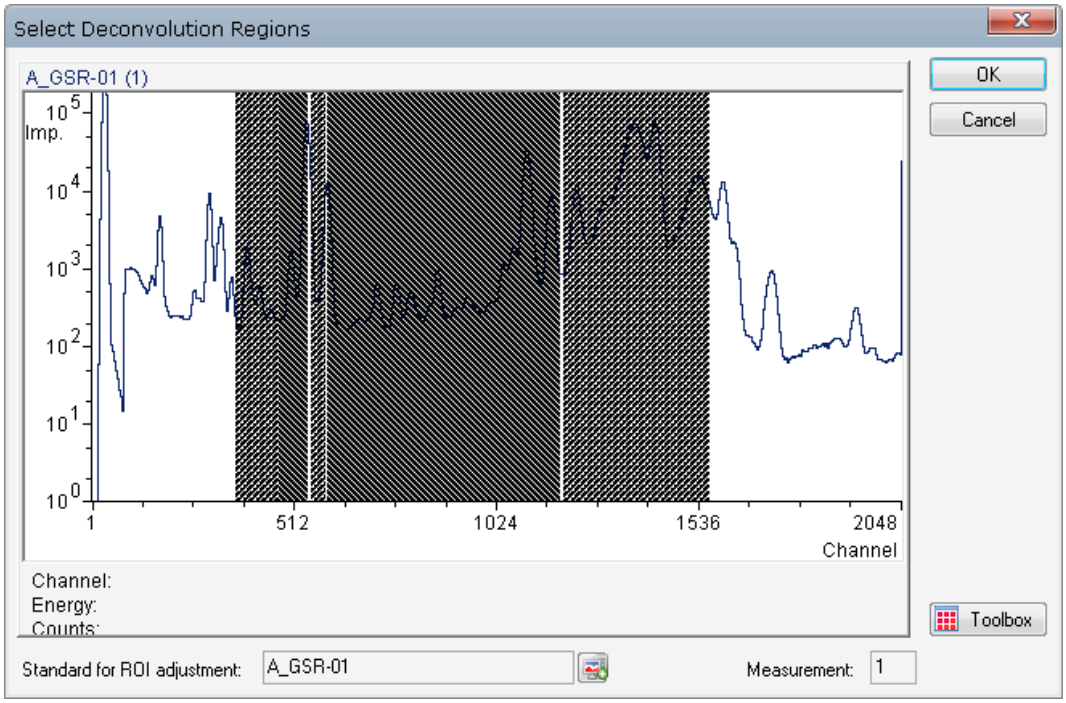
In this periodic table all elements that were selected in the tab Elements are marked in yellow and can be selected. All elements which can be excited in this sub-measurement should be selected. To select an element, click the element symbol and the colour changes to red.

All selected elements will be deconvoluted. It is not necessary to calibrate all of them or use them as concentration elements. For the Compton target it is essential to deconvolute the elements even if no concentration is calculated from the Compton target (like in most geological calibrations).
In this way the overlaps with the scattering lines can be corrected.

Only the elements selected in this PTE can be ticked as "concentration elements" in column *Conc.*

Deconvolution Region:
Most of predefined SPECTRO methods do not require any changes in the deconvolution settings. If this is required for a specific application, the Optimization must be disabled

With the above defined settings all lines to be deconvoluted are selected, but it is not defined where the lines are and in which way they should be grouped in deconvolution areas. These deconvolution areas are selected with the button Deconvolution Region. These ROIs should be created in such a way that all elements are in ROIs but not too many lines in the same ROI.

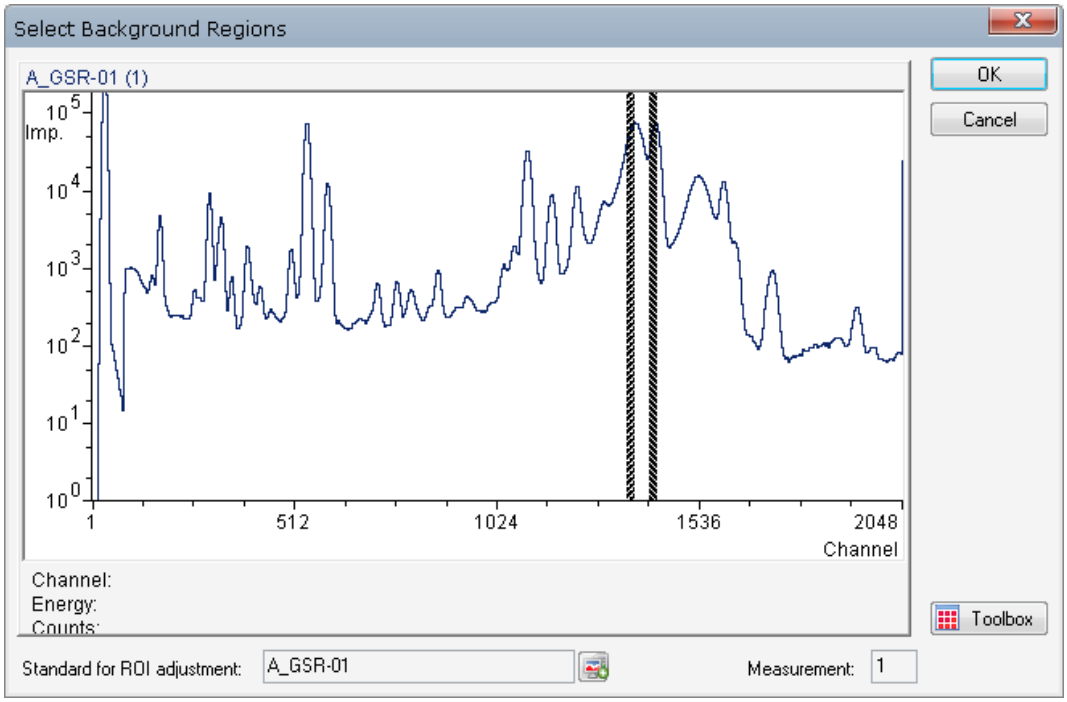


To create a ROI, the cursor is moved to the left edge of the planned ROI and then the right mouse button is pressed. When the mouse is moved to the right hand side – with still pressed mouse button – a region will be marked as ROI in a different hatching. To simplify the creation of the ROIs, it is quite useful to show the lines of the elements for this sub-measurement. This makes it easier to check, if all elements are in selected regions and if all lines of the elements with *Series Fit* are in the same deconvolution area.

To create the background regions, it is necessary to display a spectrum. The sample shown in the window can be selected at the bottom of this window. There's a list with all measured standards.

The deconvolution areas will be copied together with the rest of the parameters, when a method is copied. So, it is not necessary to edit all the regions.

Background Region:
A background spectrum can be fitted to the measured spectrum after some of the detector artefacts (as an example: pile-up, escape, shelf) have been corrected. To do this, fitting regions have to be defined, according to the way described under Deconvolution region:

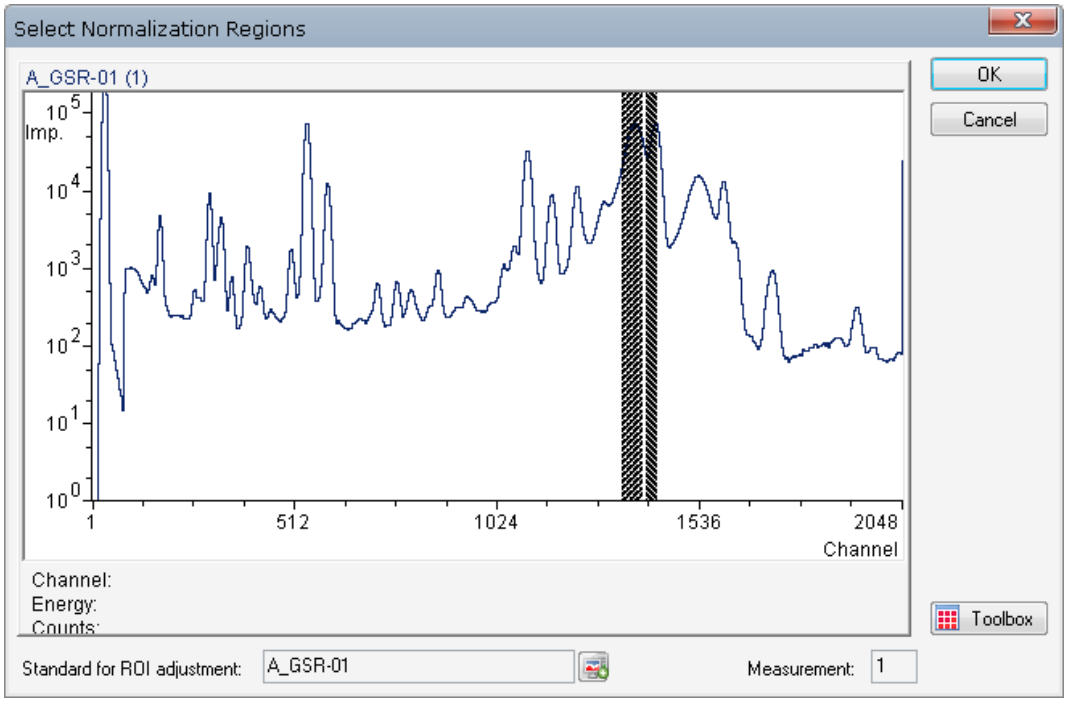


The fitting of the background spectra allows to use longer measuring times for the background spectra to reduce statistical effects. The fitting regions should never be in regions where elemental lines might influence the height of the fitted background.

Normalization Region:

The normalization regions are defined exactly the same way as deconvolution and background regions.

The normalization regions are parts of the spectra that can be used to normalize the net count rates of an element. These normalization regions are necessary for Compton targets because the entire principle of the Extended Compton model (see *Evaluation*) and of the matrix correction based on the Compton intensity (or the Compton/Rayleigh ratio) is based on this normalization:



These normalization regions can be used as an internal standard even for other sub-measurements. Two normalization regions are allowed per sub-measurement.

Iron-Cobalt-Correction:
With the button *Iron Cobalt Corr.* a special correction for Cobalt can be activated. This correction improves the determination of Cobalt traces in the presence of a large amount of iron. The correction factor should not be changed. This special correction is only possible if the Co K_α and the Fe K_β- Lines are in separate ROIs.

Use Optimization:
By ticking the *Use Optimization* check box the parameters from the three buttons *Deconvolution Region*, *Background RegionNormalization Region* are calculated automatically.

The deconvolution of a sub measurement follows the rules:

- The deconvolution areas (ROI, region of interest) are unfolded with increasing energy.
  - In each ROI, the elements with Line Fit or Line Fit with Standard will be processed with increasing energy. The K□-line (or the L□-line) will be deconvoluted and founded on the net count rate.
  - The additional lines of the same shell will be subtracted from the spectrum. For the L-series all lines of the three different sub-shells LI, LII and LIII will be considered. The coupling factors for the sub-shells can be edited in the Evaluation sub-method.
  - Then all elements with a Series Fit are deconvoluted with increasing energy.

The deconvolution parameters are absolutely essential for the proper evaluation of a sub-measurement. Wrong or missing deconvolution parameters might result in severe problems of the software.

A *series fit* is only allowed, if all lines for one specific element are in the same deconvolution area (see Deconvolution Region) and if the background under the lines is not too different.
If the background is too different, the line ratio might be influenced and this will harm the accuracy of the *series fit*.

While copying a method all of the elements, lines and even deconvolution strategies will be pre-set, reducing the necessary effort to a minimum.

33.10 Deconvolution Strategies

The deconvolution is necessary to determine the net counts for the individual elements of the method.
This can be done, using different mathematical procedures:

- Summation,
- Series Fit,
- Line Fit and
- Line Fit with Standardization

The first one is used only for special applications (e.g. during a mapping using a MIDEX equipped with xyz stages).
To explain the differences between Line Fit and Series Fit, let's have a look, what happens with a new unknown sample during its evaluation:

The energy-range of a sub-method is devided in different Regions of Interest (ROIs).
These ROIs and their contents will be calculated from low-energy ROIs to high-energy ROIs.

Starting with the first ROI, the first step will be the **Line-Fit** for all Line-Fit-Elements:
It will start with the elements with the smallest Atomic-Number. In common cases the Alpha-line like K-Alpha is chosen. In this case, the K-Alpha-line of this element will be fitted. Based on this result, the corresponding
Beta-line is calculated using a theoretical alpha-beta-ratio. After removing these lines (alpha and beta) from the spectra, the deconvolution will continue with the next element.
Doing this step-by-step (or element-by-element) all elements Line-Fit was chosen for, will be removed from the spectra.

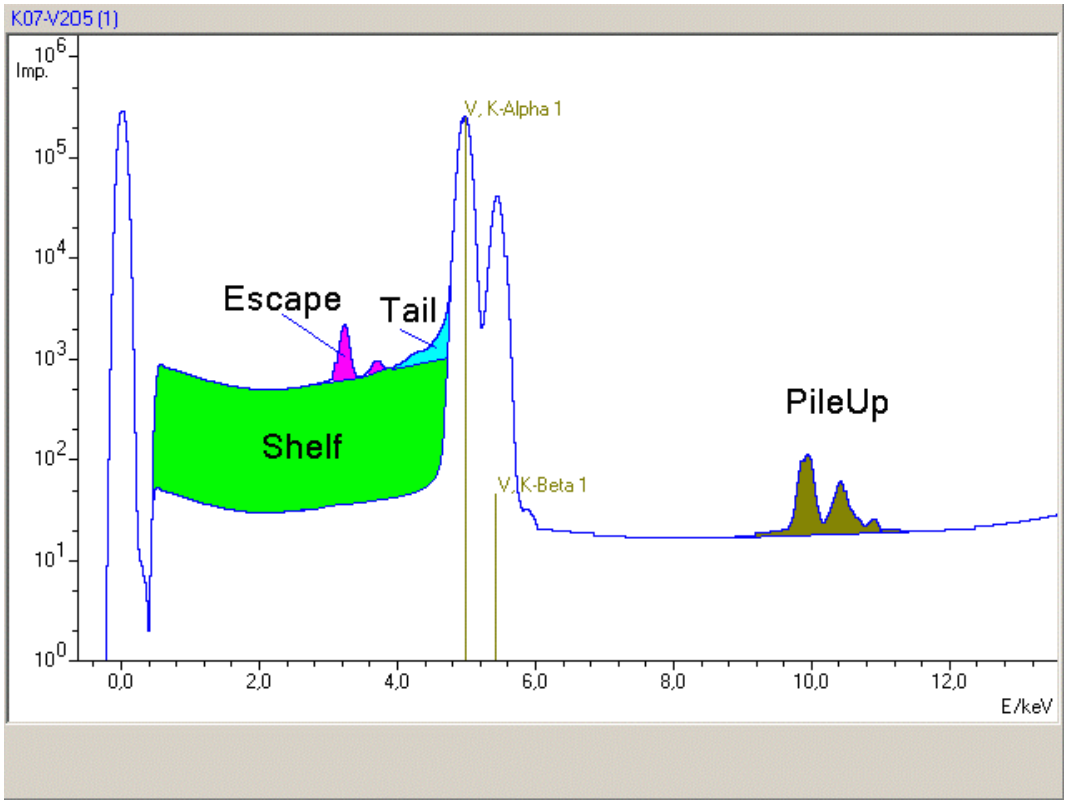
The residual spectra will be taken into a next deconvolution step:
In this last step, all elements with **Series Fit** (in one ROI) are deconvoluted in one step in a big equation-system.

Line-Fit with Standardization means that, if a minimum intensity is reached, the peak is used to recalibrate the energy-channel-calbration for this sample.

33.11 Artefacts:

The following figure shows a spectrum of the sample V2O5.
Without the artefacts the spectrum should contain the background information from the instrument and the V-lines.

But in reality the spectrum looks a little bit different than expected: In addition to the V-lines, it shows the 4 artefacts:
- Shelf
- Tail
- Escape
- PileUp



As the figure shows, SHELF and TAIL are both creating additional background at the low-energy side of a peak. Both decrease the S/N ratio with the result of increased detection limits.

If elements shall be identified manually, the artefacts described in the following are more difficult to handle, because they are creating "peaks":

The artefact Escape has an energy which is reduced by around 1,75 keV compared to the "original"-peak. That's the energy of Silicon, which is used as detector chip material.

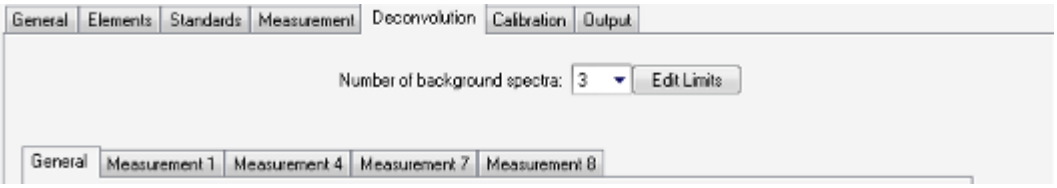
The PileUp occures, when 2 photons, reaching the detector at the same time are identified as 1 photon with doubled energy. If the "original" peak is a single peak (because peaks cannot be separated) like Si-K-series, we will find 1 PileUp peak. The figure above shows what happens with 2 lines like alpha- and beta-line: These

two lines will generate 3 PileUp lines, because 2 alpha-photons or two beta-photons or an alpha- with a beta-photon can combine.

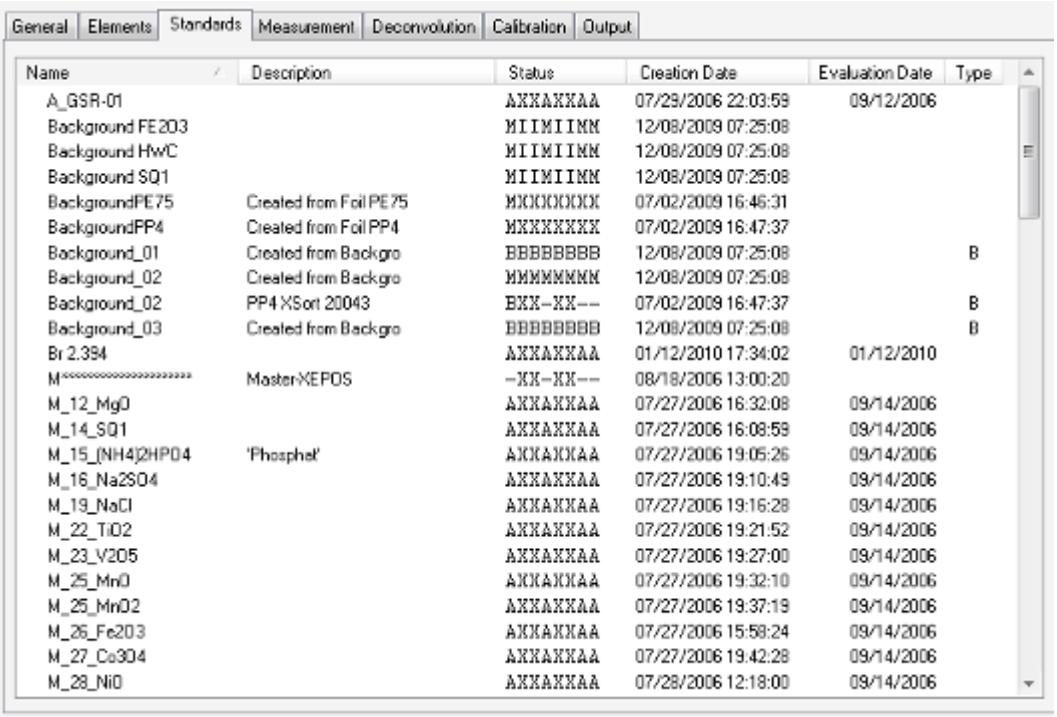
33.12 Background Spectra

One part of the evaluation of a mesurement is the subtraction of the *Background Spectra*.

For each sub-measurement up to 6 Background Spectra can be stored (Deconvolution).



That's an option, if a Compton-target like Molybdenum secondary target is used in the method.
With several background spectra available for each target it is possible to calibrate different matrices with a different scattered background (like organic and silicate samples) in one method.
Which background spectra should be used depends on the Compton/Rayleigh ratio.The background spectra are stored as standards and at the Standards they are visible as they are marked with B. Each of the shown background spectra belongs to one matrix and for each sub-meaurement a "sub-spectra" is stored:


General
Elements
Standards
Measurement
Deconvolution
Calibration
Output
Name
Description
Status
Creation Date
Evaluation Date
Type
A_GSR-01 AXXAXXAA 07/29/2006 22:03:59 09/12/2006
Background FE203 MIIMIIMM 12/08/2009 07:25:08
Background HwC MIIMIIMM 12/08/2009 07:25:08
Background SQ1 MIIMIIMM 12/08/2009 07:25:08
BackgroundPE75 Created from Foil PE75 MXXXXXXX 07/02/2009 16:46:31
BackgroundPP4 Created from Foil PP4 MXXXXXXX 07/02/2009 16:47:37
Background_01 Created from Backgro BBBBBBBB 12/08/2009 07:25:08 B
Background_02 Created from Backgro MMMMMMMM 12/08/2009 07:25:08
Background_02 PP4 XSort 20043 BXX-XX-- 07/02/2009 16:47:37 B
Background_03 Created from Backgro BBBBBBBB 12/08/2009 07:25:08 B
Br 2.394 AXXAXXAA 01/12/2010 17:34:02 01/12/2010
M Master-XEPOS -XX-XX-- 08/18/2006 13:00:20
M_12_MgO AXXAXXAA 07/27/2006 16:32:08 09/14/2006
M_14_SQ1 AXXAXXAA 07/27/2006 16:08:59 09/14/2006
M_15_(NH4)2HPO4 'Phosphat' AXXAXXAA 07/27/2006 19:05:26 09/14/2006
M_16_Na2SO4 AXXAXXAA 07/27/2006 19:10:49 09/14/2006
M_19_NaCl AXXAXXAA 07/27/2006 19:16:28 09/14/2006
M_22_TiO2 AXXAXXAA 07/27/2006 19:21:52 09/14/2006
M_23_V2O5 AXXAXXAA 07/27/2006 19:27:00 09/14/2006
M_25_MnO AXXAXXAA 07/27/2006 19:32:10 09/14/2006
M_25_MnO2 AXXAXXAA 07/27/2006 19:37:19 09/14/2006
M_26_Fe2O3 AXXAXXAA 07/27/2006 15:58:24 09/14/2006
M_27_Co3O4 AXXAXXAA 07/27/2006 19:42:28 09/14/2006
M_28_NiO AXXAXXAA 07/28/2006 12:18:00 09/14/2006

It can be necessary to modifiy these background spectra depending on the application.

33.13 Background and Contaminations

In addition to the elements in the sample, which will have to be to measured, there are some "contaminations" in the spectra, making the job a little bit more difficult.

"Contaminations" of Spectra:

The Target:
- The Target Material: Mo, Zr, Pd, Zn, CsI, Co
- The Compton-Peak: Mo-, Pd- and Zr-Target
- HOPG-Target: The tube material (anode): Pd + Reflections
- Filters: Mo, Zr, Ta, Pd, Cu, Fe

The Measuring Chamber:
- Iron

The Detector:
- Ta, Zr or Pd and a little bit of Sn (detector cooling)

All these "contaminations" together are visible in the Background spectra.

Sample Cups / Protection Film:
- Prolen: without contaminations
- Mylar: P and Ca
- Carbonat: Si

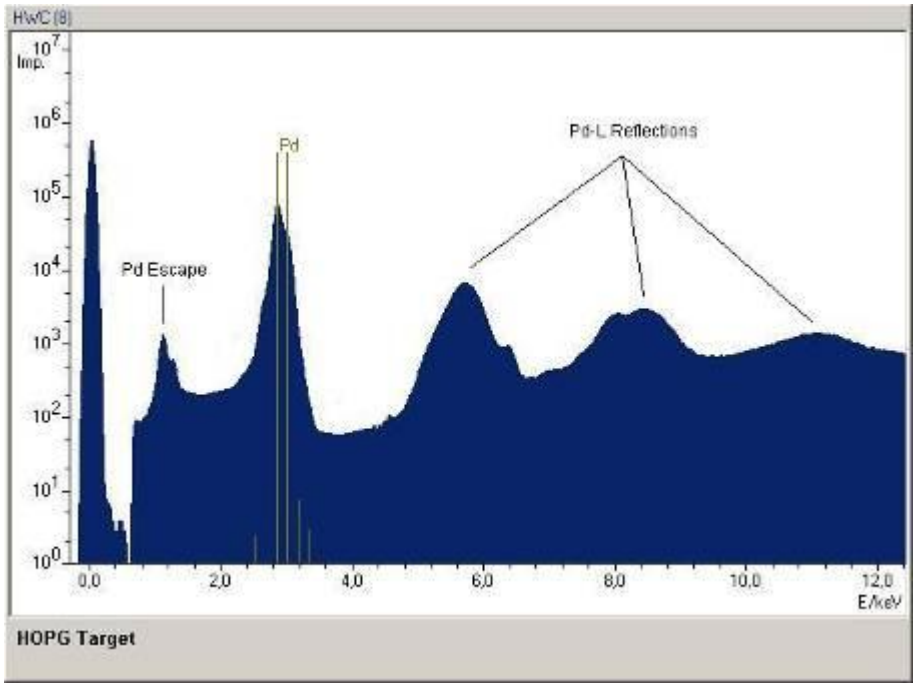
The Dilution Material:
- Oil: Sulfur
- Charcoal: a variety of elements

Artefacts

Contaminations in the instruments, e.g. after a foil crack, or caused by sample preparation

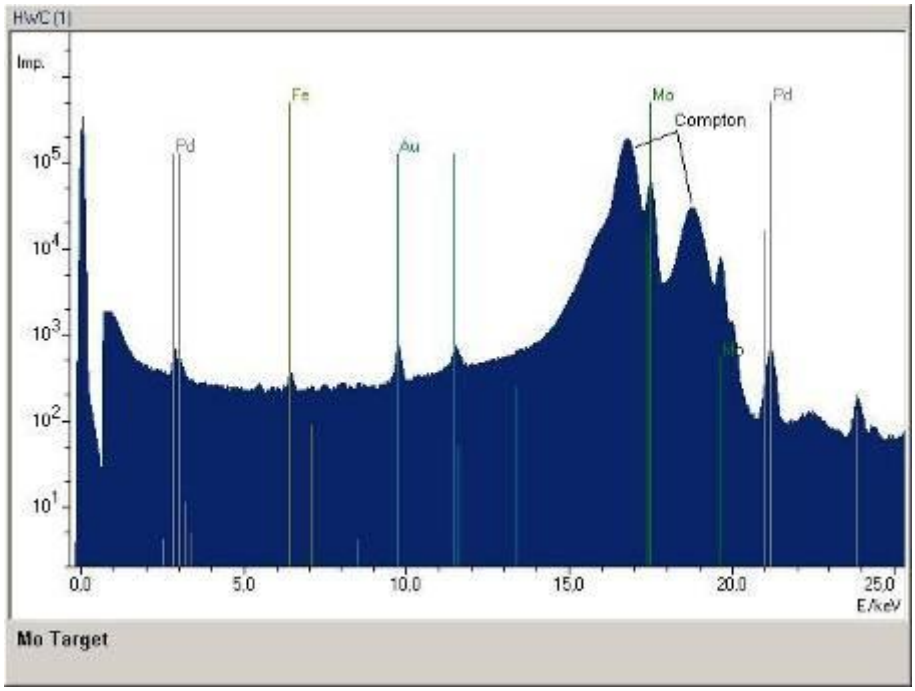
Background Spectra:

Background Spectra for XEPOS:



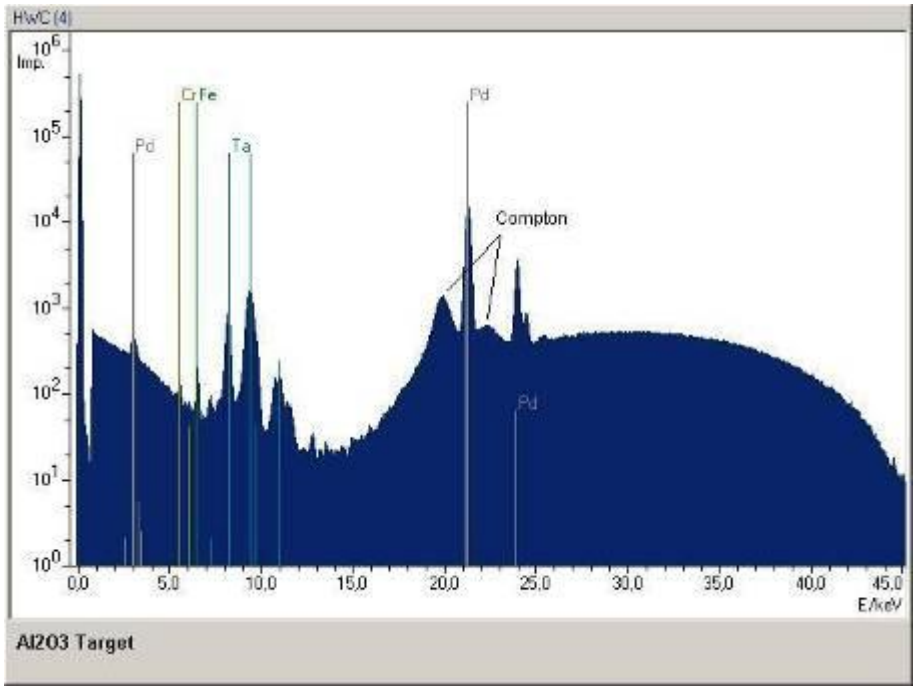
HOPG-Target

(Low-Energy range)



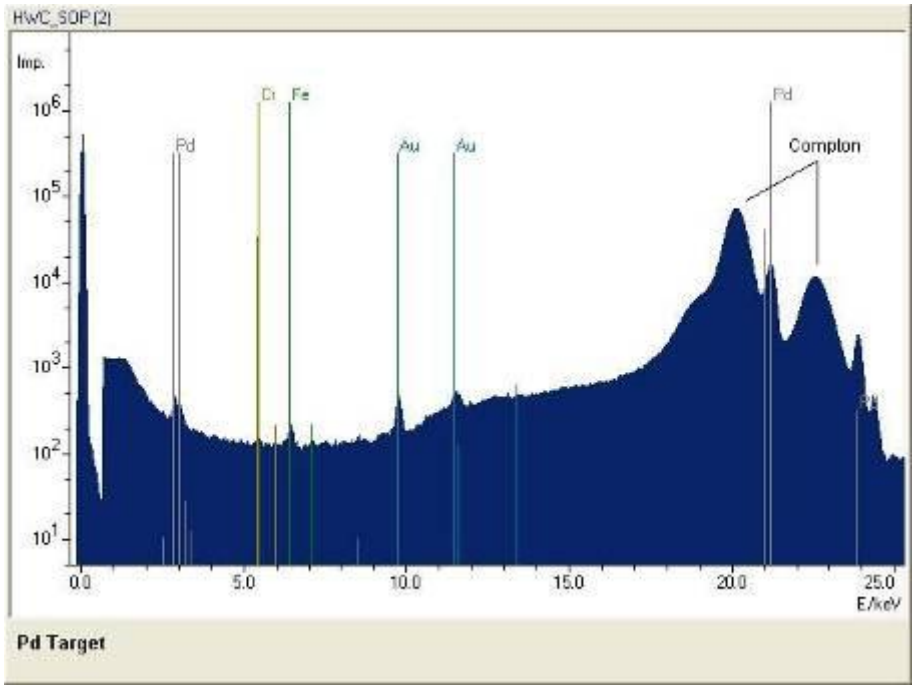
Mo-Target

(Mid-Energy range)



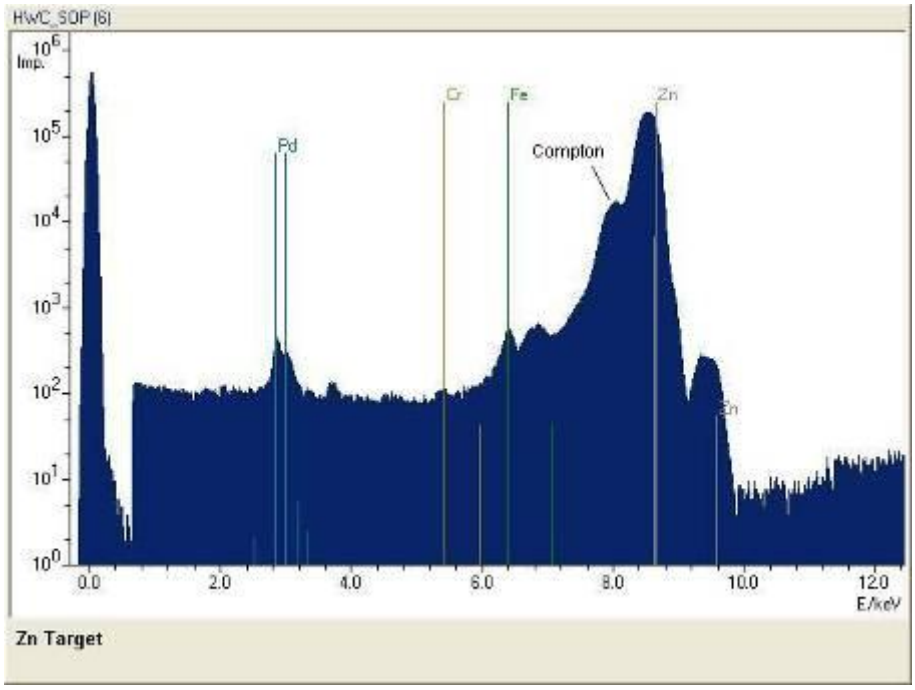
Al2O3-Target

(High-Energy range)



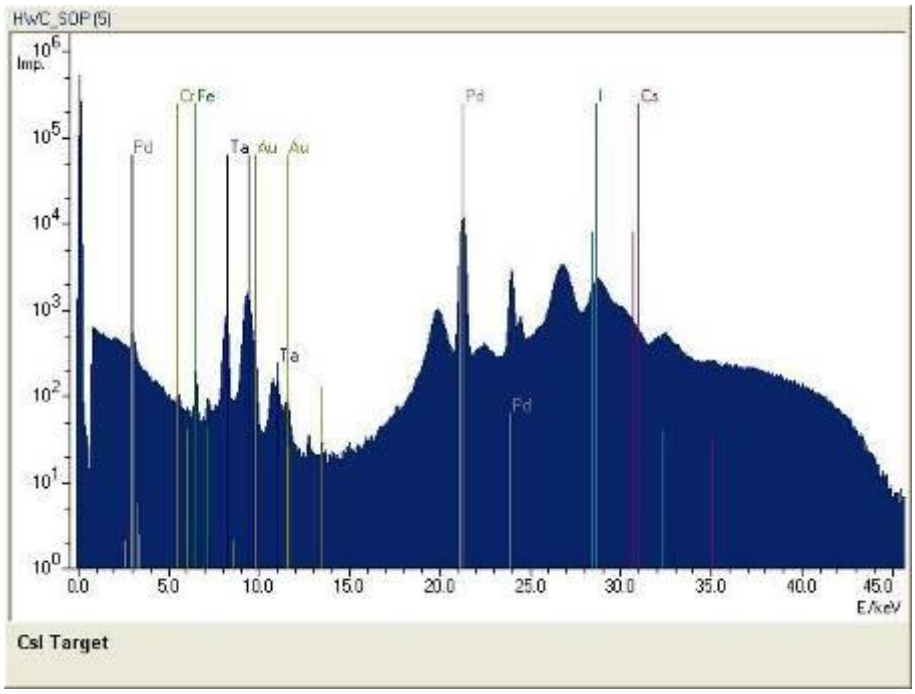
Pd-Target

(Mid-Energy range)



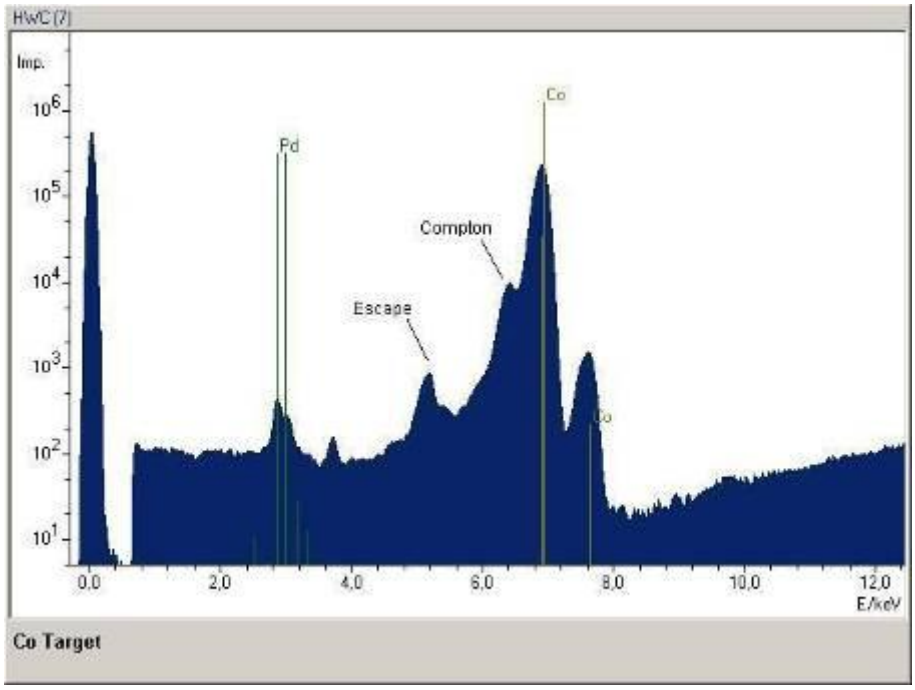
Zn-Target

(Low-Energy range)



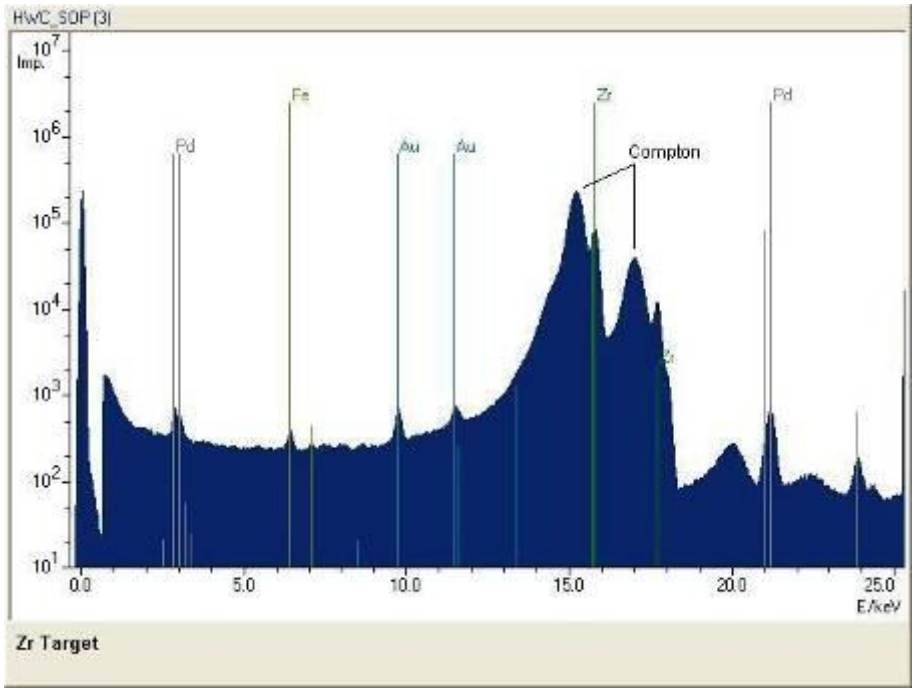
CsI-Target

(High-Energy range)



Co-Target

(Low-Energy range)

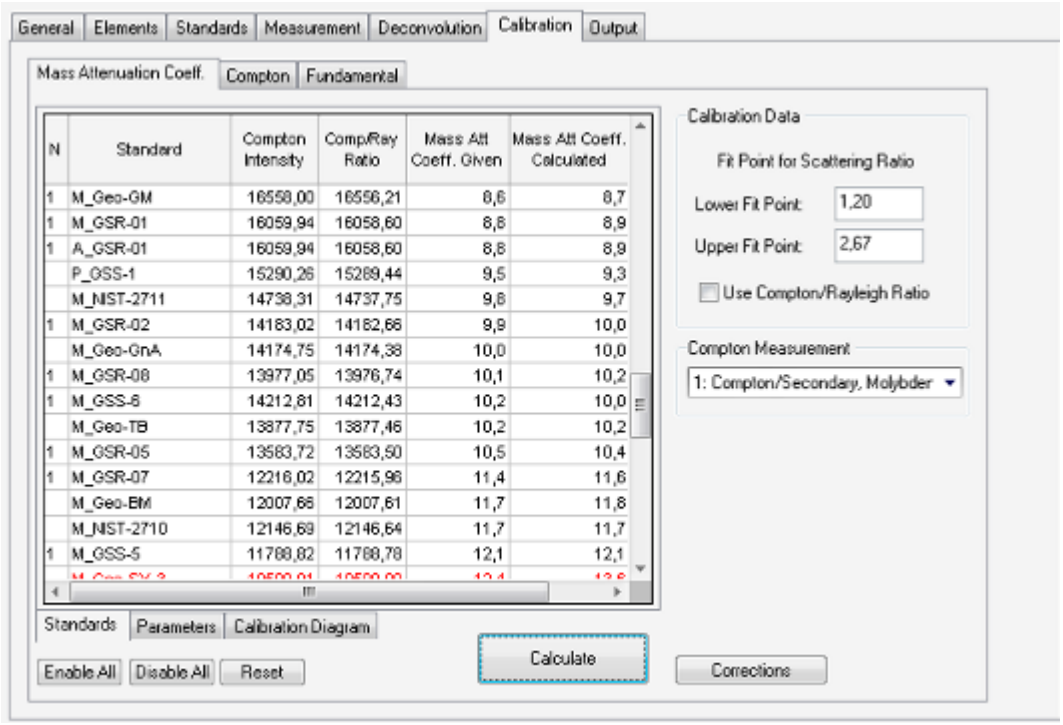


Zr-Target

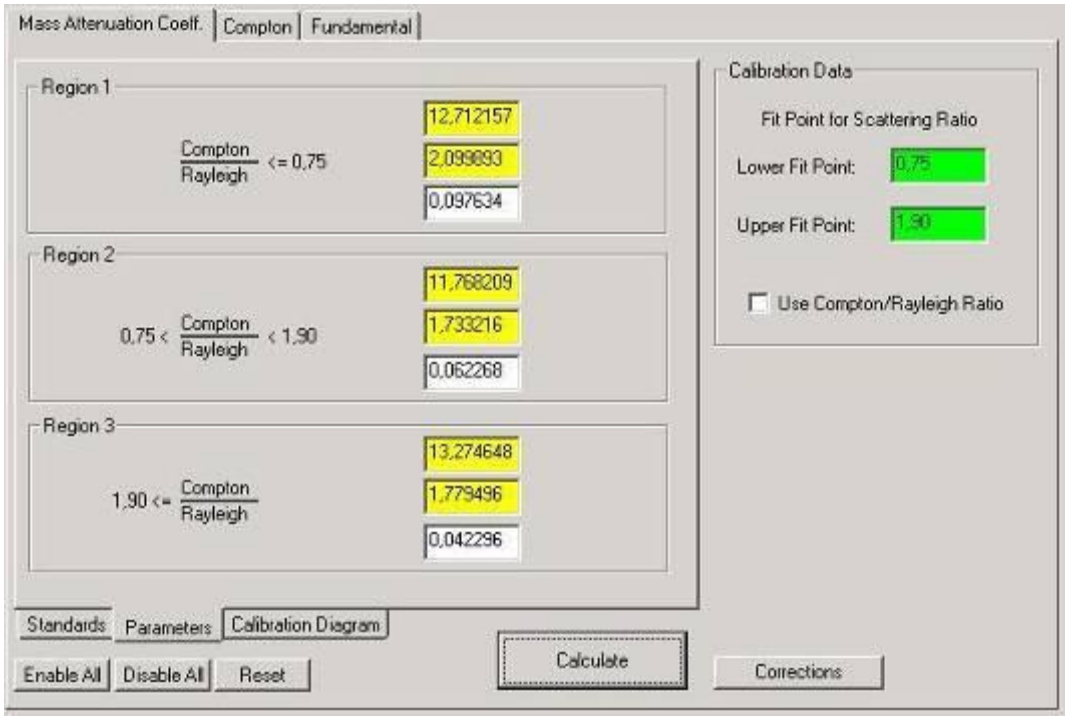
(Mid-Energy range)

33.14 Calibration of the Mass Attenuation Coefficient

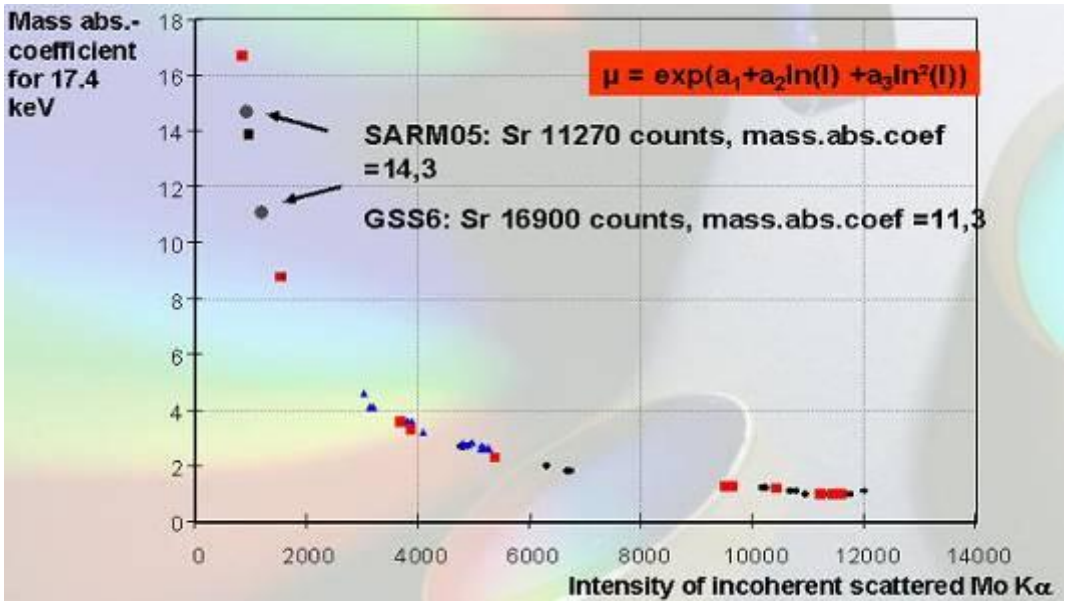
The calibration of the Mass Attenuation Coefficient is a possibility to get an impression about the size of the "non-visible" part of the sample and it is used as part of the SPECTRO procedure. To do this the Compton peak is used.



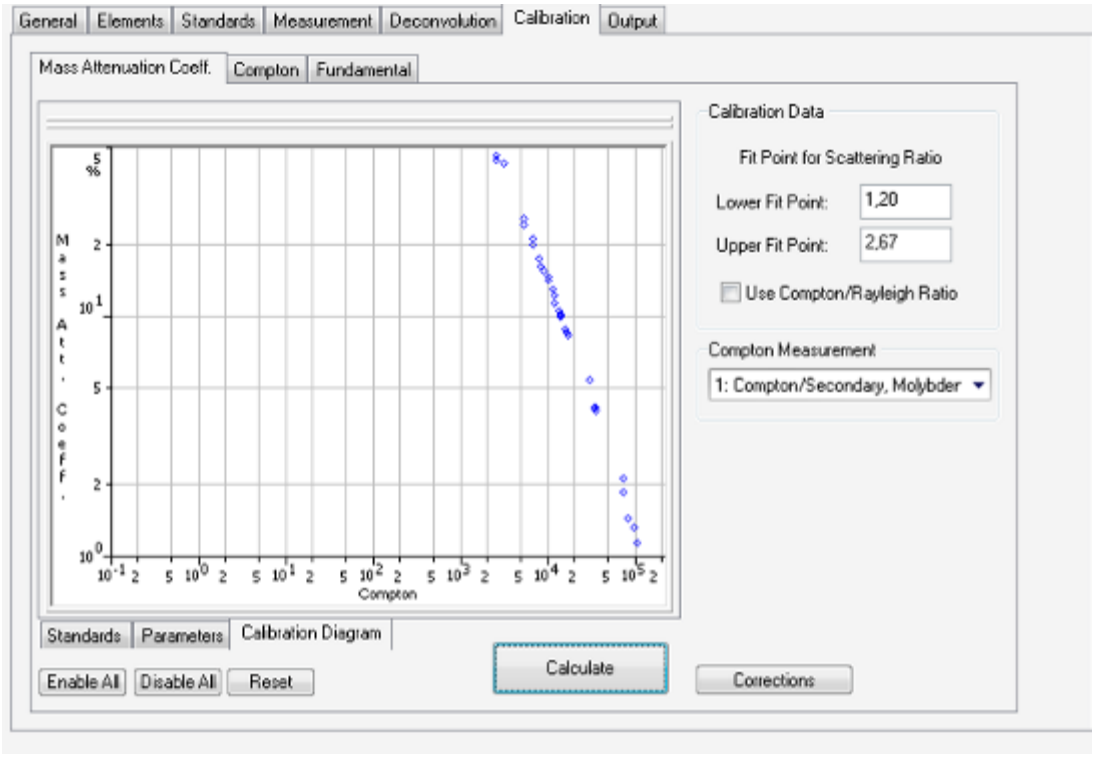
In the frame of the calibration 9 parameters are calculated. Look at the tab Parameters (see figure below).
The green highlighted limits are the switch-limits for the three regions.
If these parameters shall be controlled, the yellow highlighted parameters should be positive.



The following figure shows the correlation between Compton intensity and "mac". a1, a2 and a3 are the three parameters for each region (1 to 3) shown in the figure above, "I" means the intensity of the Compton peak and μ is the "mac".

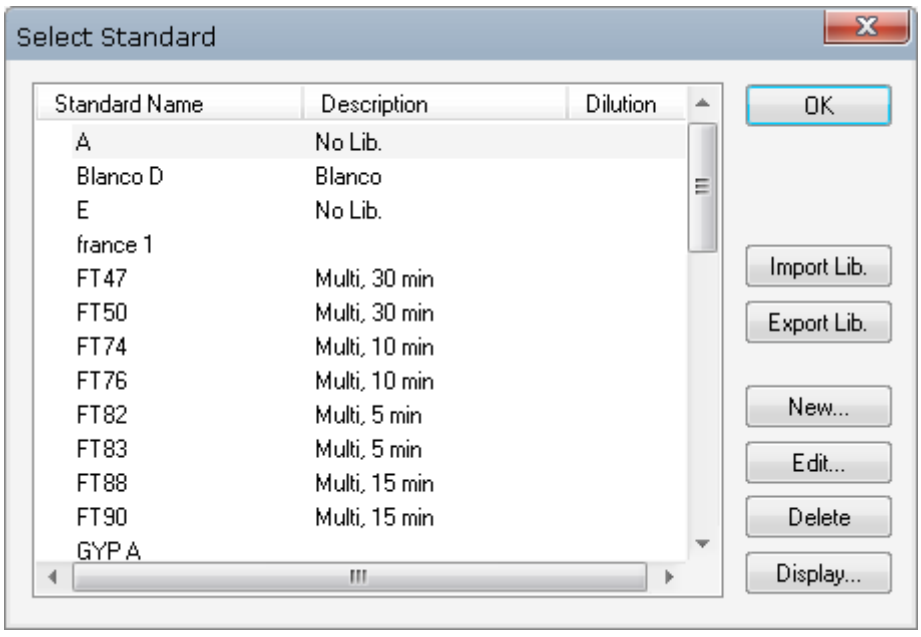


For a better visualization a double logarithmic scale is used to form a diagram in the tab *Mass Attenuation Coeff*. The expected result is a line.



33.15 Library of Standards

The Library of Standards is available in the menu *Tools*.



It is a database which contains the given concentrations of a lot of Certified Reference Materials (CRM). These data should be used during the creation of new samples used as standard:

It is much faster done, if the given concentration were copied/imported from this database instead of entering each element concentration.

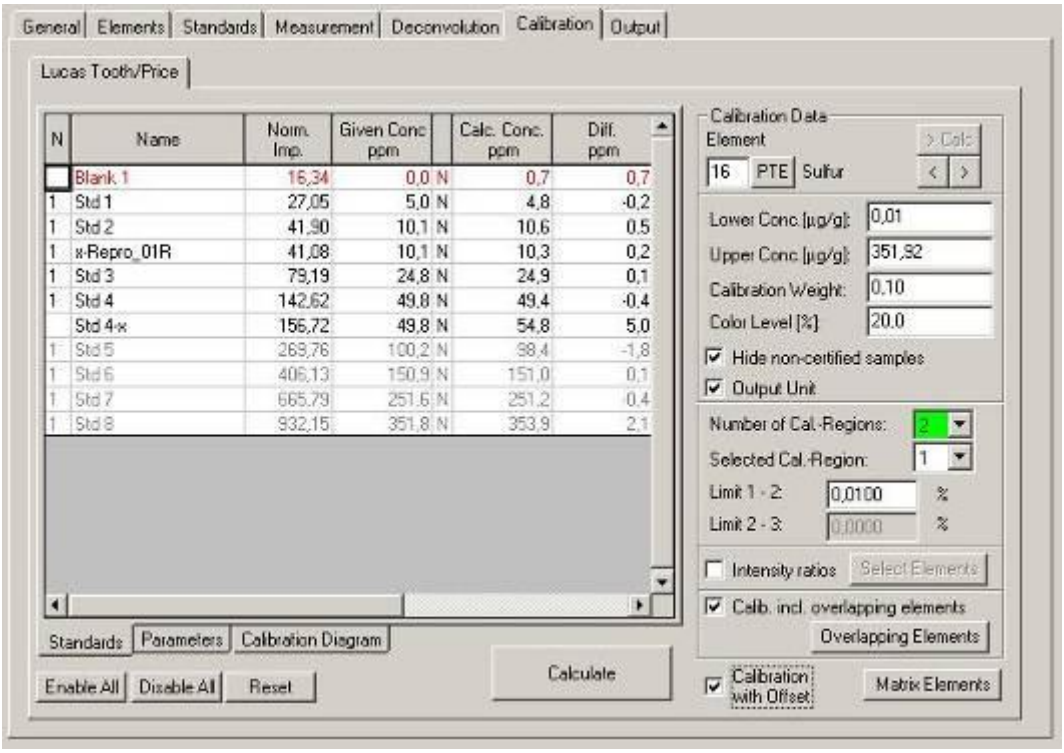
33.16 Regions in Lucas-Tooth/Price

The Lucas-Tooth/Price calibration is the only one, which supports more then one calibration region.

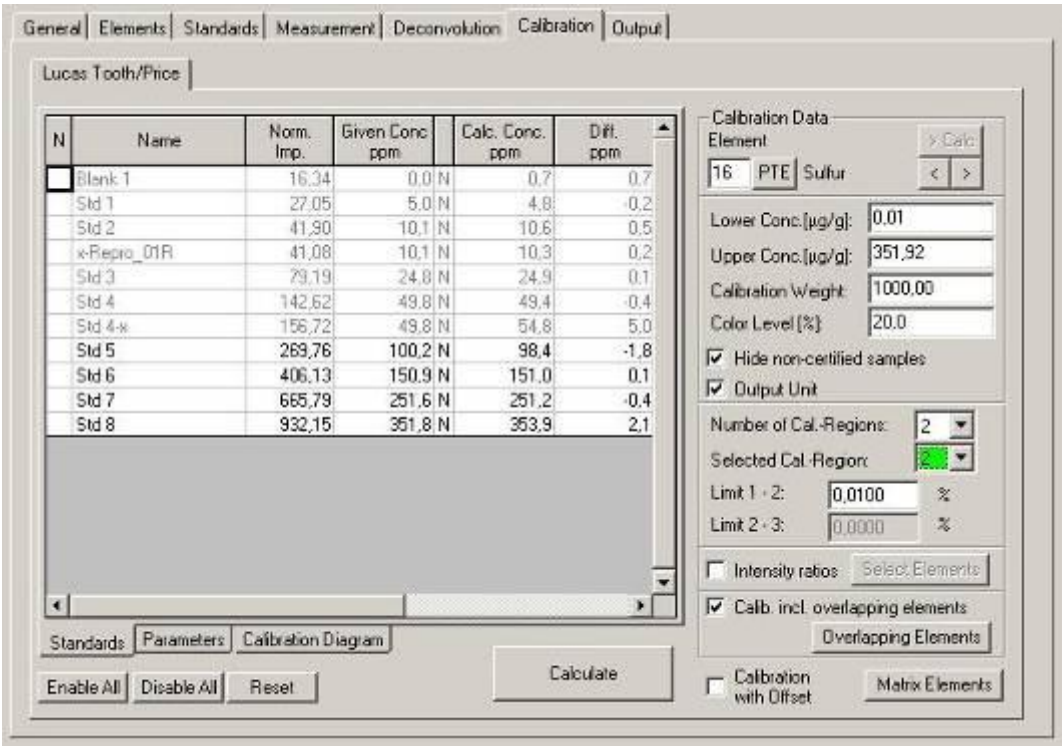
This feature can be used, if the concentration range is too big to get good results.

An example is Sulfur in Diesel. There are two possible regions:
- Around 400 ppm of S as common region and
- smaller then 10 ppm of S for Low-S-applications.

This example is used to show the region-feature.
First of all, the number of regions has to be increased. Doing this, the parameter "Limit 1 - 2:" is used to define the switching-limit. That's the concentration, where the next region (in this example region 2) starts. In the figure below, the limit is 10 ppm, that means, that for concentrations smaller then 10 ppm region number 1 is used and for higher concentrations region 2:

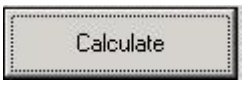


Pressing "Calculate" will calibrate only region 1!
The "Selected Cal.-Region:" shows, that the list at the left side is presenting the samples and results for region 1.
If the second region (> 10 ppm) should be calibrated, change the "**Selected Cal.-Region**" into "2":



After this change, pressing "Calculate" will calibrate the second region.

33.17 Error Messages during Calibration

After pressing 

some error messages can appear, if something unusual was calculated.

Following a summary of these messages:

Message	***Reason***	***Solution/next step***
Negative Offset	A negative Offset was calculated	**Remove** the Offset option
Offset seems to be too big	Offset is unexpected big	If the reason can be found and explained, the message can be ignored (1)
Incorrect correction	The calculated correction cannot be explained by Physical laws	**Remove** the mentioned element
Negative	The calculated correction	**Remove** the mentioned

correction	cannot be explained by Physical laws	element
Unexpected correction	The parameter for the correction is unexpected big.	If the reason can be found and explained, the message can be ignored (2)
No. of Standards too low	Too many corrections No samples selected	More samples or less corrections (including Offset) "Enable" samples
Negative Slope	The slope of the calibration line is negative	Many times, there is an error in the given concentration like a wrong unit during definition. **Has to be removed**

Known examples for error messages which can be explained / ignored:
(1) "Offset seems to be too big" If the detector has a Zirconium collimator, the offset for Zr will generate this message - that's ok.
(2) "Unexpected correction" Some K- and L-series line-overlappings like Ba-L and Ti-K are creating these messages, if they are corrected.

34 Important Information

Data Backup

Regular data backups are important for the operation safety and availability for your analytical system. Utilities that enable regular backups of the program directory that are appropriate for the installed operating system should be used. In this way, it is possible to restore the most current data possible to a new computer or newly installed software if the PC or your specific data is lost or destroyed. The medium on which the backup is stored should be stored in a location that is spatially separated from the PC.

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